Projecte de Fi de Carrera
**Enginyer Industrial**

# Design of a sustainable urban vehicle

Memòria


Autor:
**Daniel Caballero**
Director:
**Daniel Montesinos**

Convocatòria:
**Setembre 2016**


Escola Tècnica Superior d'Enginyeria Industrial de Barcelona

**Abstract**

Transport is a great consumer of energy and a great emitter of GHG. Moreover, in cities where the population is more concentrated other issues arise due to transport. To tackle these problems, the cradle-to-gate and well-to-wheels life cycles of different vehicles are analysed. Then, a choice of the most sustainable option regarding energy consumption and GHG emissions is made. Finally, the control system of the chosen one will be designed.

**Resum**

El transport és un gran consumidor d'energia i un gran emissor de gasos d'efecte hivernacle. A més, a les ciutats, on la població està més concentrada, d'altres problemes sorgeixen. Per mirar d'atenuar aquests problemes, analitzem el cicle de vida de vida de diferents tipus de vehicle—tant del vehicle com el combustible—. Dels vehicles analitzats, es triar el més sostenible, en termes de consum d'energia i emissions. Finalment, es dissenyarà el sistema de control del vehicle triat.

# Contents

# Introduction

## Motivation

The world's population is increasing. While there is no consensus on how this trend will evolve in the future, there is on where will we live: the urban population in 2014 accounted for 54% of the total, up from 34% in 1960. Moreover, the urban population growth is higher in the less developed regions of the world and it is expected that by 2017 the majority of the population of those regions will live in urban areas.

Also, the demand for private transportation is also increasing in developing economies. Even though it is obvious that we live in a finite planet, the development of societies seems to always head us towards resource-exhausting, environment-polluting economies.

There is strong evidence that the resources upon which modern economies depend are nearly depleted or soon will be. For instance, conventional oil is thought to have peaked in the last decade; it is clear, then, that its increasing demand cannot be physically satisfied, so cannot an increasing demand of oil-derived-driven vehicles.

## Purpose

The purpose of this thesis is to find the most sustainable—in terms of both energy and materials—propulsion system for an urban vehicle and design its control system.

## Scope

It covers both the cradle-to-gate and the well-to wheels life cycles, that is, not only the operational energy of the vehicles, but also the energy needed to obtain the materials, manufacture the components, and assembly the vehicle. The final design of the vehicle includes models of the powertrain, with longitudinal dynamics and the control structure of the vehicle.

# Chapter 1

# State of global resources

Resources are sources or supplies from which benefit is produced. In this context, they are mainly energy and materials, but also land, water, etc. A scarcity of any of those resources can be threatening to our societies, so assessing the state of the resources upon which we depend is essential to discern wether we are on the right path; and otherwise, to know the direction of the actions we have to take.

Therefore, the purpose of this section is to give a general idea of the state of global resources. How much essential resources are left, how much energy can we produce, which energy sources are best, etc.

Since it is virtually impossible to evaluate all of the resources, we will focus only on energy resources. Also, an outline of the materials used in automotive applications, and the energy consumption associated to their production will be given.

## 1.1 Generalities

### 1.1.1 Renewable and non-renewable resources

Resources can be either renewable or non-renewable. Renewable resources are replenished within a human timescale, whereas non-renewable ones take longer amounts of time or cannot be replenished at all. It is not an intrinsic characteristic of the resource, but rather how it is used. For instance, water is a renewable resource for steam turbines, but as a source of hydrogen for nuclear fusion is a non-renewable resource.

As our economy strongly relies on non-renewable resources, such as fossil fuels, it is necessary to know how much of the resource is left. However, natural resources are not generally found in bounded *pools*, but they are found unevenly distributed in different concentrations. Plus, even more interesting than how much is left is the question of how much can we extract. On the other hand, renewable resources are not limited by the total amount of energy, but by the amount of available power.

### 1.1.2 Energy and materials cost

The process to deliver energy to the final consumer requires energy itself. For instance, to deliver petrol oil needs to be extracted, then refined and finally delivered from the well to the station. The ratio between the energy extracted and the energy needed to extract it is very useful to compare energy sources, and it is called *Energy Return On Investment* (EROI).

The available values of EROI are usually standard values, which only account for direct energy costs—site preparation, drilling, mining, pumping, etc., and site dismantling—and indirect energy—energy required to make the products used on site but produced off site, such as cement, steel forms, machinery, etc—. This calculation is applied to fuel at the point where it leaves the production facility: *mine-mouth* for mineral resources, *well-head* for liquid or gaseous resources, *wire* for electricity, etc. Then, all the associated costs should be added, such as refining or distribution.

### 1.1.3 Limiting factors to energy production

In the case of renewable resources, the limiting factor is not the total amount—energy, in the case of energy sources—but its capacity—power, resp—. Since virtually all renewable energy ultimately comes from the Sun, an upper boundary would the radiation the Earth receives. Or even, in a imaginary future, a Dyson sphere could gather most of the energy coming out of the Sun. Obviously, this is far from possible today. In fact, we are only capable of capturing only a little fraction of the energy the Earth receives. Other limiting factors are fertile land—e.g. for biofuels—, water, availability of certain materials, etc. But, as mentioned before, those other limiting factors are not analysed here.

Since the production of renewable energy depends on certain materials, one might think that it also has to have an upper limit. In that case the depletion of those materials would make it impossible to continue to produce energy. The recycling of the totality of materials would eliminate this problem, but this also has been argued impossible as a consequence of the second law of thermodynamics, or what is called the *fourth* law of thermodynamics. However, Ayres [**?**] showed that there is no such thing as a fourth law of thermodynamics and that total recycling is indeed possible for an industrial society given certain conditions, just as it occurs naturally in the biosphere.

Non-renewable resources are not limited by the amount of power available. By definition, non-renewable resources are limited by the total amount of that resource than can be extracted. However, this total amount is neither known nor precise. For one particular resource, the total amount found in the Earth's crust is known as its *resource base*. This value is of little relevance, since the most part of the resource base is not economically recoverable, is not discovered yet or might not even be discovered ever. The share of the resource base that is economically recoverable is called the *resources*. Finally, *reserves* are those resources that are proven and can actually be extracted with great confidence. In particular, the oil industry uses three categories for resources. Proven reserves are *1P reserves*, proven plus probable reserves are *2P reserves*, and proven plus probable plus possible reserves are *3P reserves*.

Because of how oil and gas are found in geological formations, not all of them can be recovered. The total amount of oil or gas in a reservoir is called *oil-in-place* or *gas-in-place*, respectively, or more generally *hydrocarbons initially in-place* (HIIP). The ratio of the reserves to HIIP is called the *recovery factor* (RF), which usually ranges from 1 to 85 percent [?] for oil. It largely depends on the geology of the reservoir, so it is difficult to increase it, even when technology evolves.

Finally, *ultimate recoverable resources* is the total amount of the resource extracted at the end of life of a well or mine. It can also be used to estimate the total amount of a particular resource that can be extracted.

Still, the amount of a resource left gives little information about how much time this resource can be made use of. Usually, to give an idea of the time that this resource will be present the *ratio of reserves to annual extraction* or *range* is used. It is simply the ratio of the proven reserves, or sometimes the resources, to the current annual rate of extraction. However, not only this ratio is a very poor indicator for forecasting, but it is confusing. Resources are not depleted suddenly, but their production follows a steep curve after its peak production, and extraction rates are not constant.

**Hubbert's peak theory**

A more accurate model for resource depletion is the Hubbert's peak theory. Hubbert [?] observed that the production of individual oil wells followed a bell-shaped curve, and predict the US oil production. The models and mathematics behind this phenomenon have since been developed and become more sophisticated, but the basic idea behind them remains. The initial theory has been extended from regional oil production to world-wide oil production. Also, the same model have been applied to other natural resources, such as natural gas, uranium, and even material resources. The theory is based on two basic assumptions, which are more than obvious:

1. There is a finite amount of non-renewable resources.

2. The resources that have not been discovered cannot be extracted.

There is debate over the suitability of this model, because it is not clear what drives this particular pattern. A more intuitive approach is to look at the discovery rate. When a resource becomes of interest, its extraction begins. As technology is developed and social demand grows, the rate of discovery increases. Since the amount of that resource is finite, the discovery rate must reach a peak. As the more easily reachable resources have been already discovered, the less accessible resources are more appealing, but they are more costly, and thus the discovery rate declines. Lastly, the discovery rate becomes zero when all the resources that are economical to find have been discovered.

There are regional discovery curves that are asymmetrical, but if there is a large population of fields, the sum of asymmetrical curves become symmetrical under the Central Theorem of Statistics [?].

The actual extraction rate curve follows the discovery rate curve after a lag time. This time lag depends on the time of setting up the extraction facilities, and the demand of that resource. If the time lag were constant, the extraction rate curve would be symmetrical as well. However, if the technological advances permit lower times between discovery and extraction, or the demand is increasing faster than the extraction rate, the lag time may decrease. Then, the extraction curve becomes skewed forward, in what is known as the Seneca effect.

This model has an important flaw, though. It does not take into account artificial disruptions that may occur. Such disruptions are, mainly, political events. The promotion or discouraging of the consumption of a resource might alter its discovery curve or alter the lag time between discovery and extraction; other events might even halt the production altogether. To model this, several curves may be used, and are indeed necessary to model global extraction dynamics. Multiple-curve models also describe technological advances that allow the discovery of resources undiscoverable with the old technology.

The curve used to model the extraction—and discovery, too—is the derivative of the logistic curve, which is known as the Hubbert curve. The equation of this curve is [EQUATION]

$$q(t) = \frac{2\,q_{max}}{1 + \cosh\big(b\,(t - t_m)\big)} \tag{1.1}$$

where $q(t)$ is the rate of extraction at time $t$, $q_{max}$ is the peak extraction, $t_m$ is the time at which peak occurs, and $b$ is a factor describing the slope. Since there are two parameters in this equation [EQUATION], it is impossible to accurately fit a curve to actual production rates. However, there is a relation [EQUATION] between those two parameters and the ultimate recoverable resources $U$. There are estimates of the value of the ultimate recoverable resources, so we only need to tune one parameter to fit the curve to the data.

$$b = \frac{4\,q_{max}}{U} \tag{1.2}$$

### 1.1.4 Sustainability

Before assessing the sustainability of a vehicle, sustainability needs to be defined quantitatively. Starting from the obvious *qualitative* definition of sustainability—that can be sustained indefinitely—we can look for factors that make something unsustainable. On the one hand, if it consumes something limited by nature, it is unsustainable. On the other hand, if it alters the environment so that at one point the damage is irreversible, it is unsustainable. The former statement can be quantified by the non-renewable resources consumed. The latter, by the amount of pollution it emits.

#### Non-renewable energy consumption

To the equivalent amount of non-renewable energy from the total energy we define the *depletion factor* ($d$), which is simply the ratio between total non-renewable energy consumption and energy consumed [EQUATION]. It can be more than one, because of the upstream energy consumption associated with the particular source.

$$d = \frac{E^{total}_{non-renewable}}{E_{consumed}} \tag{1.3}$$

If an activity—for instance driving a car—involves a chain of actions $i = 1 \dots N$, which consume an amount of energy $E_{i.j}$ from a set of $j = 1 \dots M$ energy sources, with an associated depletion factor $d_j$, the amount of non-renewable energy consumed $E$ by that activity will be:

$$E = \boldsymbol{s} \cdot \boldsymbol{E} \cdot \boldsymbol{d} \tag{1.4}$$

Where $\boldsymbol{E} = \{E_{i,j}\}$ is the matrix of energy consumptions, $\boldsymbol{d}$ is the column vector of the depletion factors, and $\boldsymbol{s}$ is a vector of $M$ ones, used to perform the sum.

### Greenhouse gases emissions

The pollution does not only cause global warming, so it would be unrealistic to reduce the pollution to greenhouse gases emissions. However, global warming is of much concern, and the data is easily accessible. It would be impossible to take all the harmful emissions into account, so we will focus only on greenhouse gases. Furthermore, there are a lot of gases that produce the greenhouse effect, but we will only look at the three main greenhouse gases (GHG) emitted by transport-related activities. Those are carbon dioxide ($Co_2$), nitrous dioxide ($NO_2$) and methane ($CH_4$).Each of those gases have different effects on the global temperature, so the *global warming potential factor* (GWP) is used. GWP is a measure of the greenhouse effect a particular gas produces compared to carbon dioxide in a time span of one hundred years. The GWP of the three gases mentioned before are listed in [TABLE]

Table 1.1: Global warming potential factors [**?**]

| Gas | 100-years GWP |
|---|---|
| $CO_2$ | 1 |
| $CH_4$ | 25 |
| $N_2O$ | 298 |

Similarly to the non-renewable energy consumption, to calculate the GHG emissions ($G$) of an activity we will use the expression [EQUATION].

$$G = \boldsymbol{s} \cdot \boldsymbol{E} \cdot \boldsymbol{\varepsilon} \tag{1.5}$$

$$\varepsilon_j = \sum_k \mathrm{GWP}_k \cdot \varepsilon_{j,k} \tag{1.6}$$

where $\varepsilon_{j,k}$ is the emission factor of the gas $k$ associated with the activity $j$.

**Corrected energy consumption**

The complexity of the climate system makes it very difficult to accurately estimate the effects of GHG emissions. Even though it is possible to guess which are those effects— rising sea levels, draughts, extreme weather, dispersion of tropical diseases, etc.—, quantifying and putting them in a time scale proves to be a much more arduous task. Instead of trying to make a model, we can combine the energetic cost of the mitigation of those effects with the energy consumption. To do so, the social cost of carbon (SCC) is used.

Social cost of carbon is an estimation of the economic cost of the mitigation measures of the effects of global warming. It is used as an estimation of the value a carbon tax should have, that is, to account global warming as an externality. The conversion of the SCC into energetic units is treated in the [APPENDIX].

The conversion of GHG emissions into energy units is even more valuable since it allows us to use a single parameter to compare different options. This parameter is the corrected energy consumption and is calculated using the [EQUATION].

$$E_c = E + \mathrm{SCC} \cdot G \tag{1.7}$$

## 1.2 Energy sources

In this section, the energy sources are analysed. First, for non-renewable energy sources, the data of extraction rates is fitted to a single or multiple Hubbert curves, what it is best. Then, the depletion and emission factors are calculated for each source. For renewable sources of energy, the evolution of installed power is analysed, and the data is fitted to a logistic curve. To do so, the upper limits of the production of renewable energy given in [**?**] are used. Those limits are supposed to be safe limits, that is, that do not deplete the material resources reserves, and do not notoriously alter the environment. Finally, a forecast of the future production of energy is given, as well as an estimation of the fraction of that energy that can be used in transport.

### 1.2.1 Coal

Coal is an organic sedimentary rock composed chiefly of carbon along variable amounts of hydrogen, sulphur, oxygen and nitrogen. It occurs in rock strata in veins called coal seams. It is used for power generation and as a feedstock for several industrial processes including steel and cement manufacturing.

Coal formation began in the Carboniferous, between 345 and 280 million years ago. Coal forms from the accumulation of organic matter, mostly plant debris, which undergo several changes as a result of bacterial decay, compaction, heat, and time. To become coal, the accumulation of debris must be greater than the rate of bacterial decay. In swamps where the water level remains constant for long periods of time this condition is met, since the standing water prevents the debris from decaying. After a certain amount of time, these debris become peat. Once a thick layer of peat is formed, the build-up of sediments together with tectonic movements bury it. Heat and pressure will transform the peat into coal in a process known as coalification. The quality of coal largely depends on the type of vegetation it originated from, the depth of burial, the temperatures and pressures at that depth, and how long it took the coal to form. These factors determine the degree of transformation, or rank. There are four ranks of coal:

**Lignite** is the youngest form of coal and is usually referred to as brown coal due to its brownish colour. It is mainly used for power generation and accounts for 17% of the world's reserves. Its lower heating value is around 17 MJ/kg, with a carbon content between 60–70% .

**Sub-bituminous coal** is the next stage of coalification. It is used for power generation and several industrial processes. It represents 30% of coal's reserves. Its carbon content is around 71–77% , and its lower heating value ranges between 19–26 MJ/kg.

**Bituminous coal** is a high quality coal (its carbon content ranges between 77% up to 87%). It is the most abundant form of coal and comprises 52% of reserves. It is used for power generation, cement manufacturing, and other industrial processes—thermal coal—and for manufacturing steel—metallurgical coal—. Its lower heating value is between 24–33 MJ/kg.

**Anthracite** is the highest rank of coal. It consists of over 87% of carbon and up to 98%. It has the highest heating value, near 35 MJ/kg. However it is the most scarce form of coal, as only represents 1% of global reserves.

### Production model

The production model of coal consists of three Hubbert curves. The data is taken from [**?**]. The model assumes an ultimate recovery of $U = 600\,\mathrm{Gtoe}$ [**?**]. The parameters of the curve are listed on [TABLE].

Table 1.2: Coal curves' parameters

| Curve | $b$ | $q_{max}$ | $t_m$ |
|---|---|---|---|
| 1 | 0.2553 | 665 | 1986 |
| 2 | 0.1517 | 1607 | 2018 |
| 3 | 0.0288 | 4514 | 2067 |

The data and the fitted curve can be seen on [FIGURE]. The fitted model has an $R^2 = 98.05\,\%$.

### Coal depletion and emission factors

The detailed calculation of coal's depletion and emission factors can be found in [APPENDIX]. The results are shown in [TABLE].

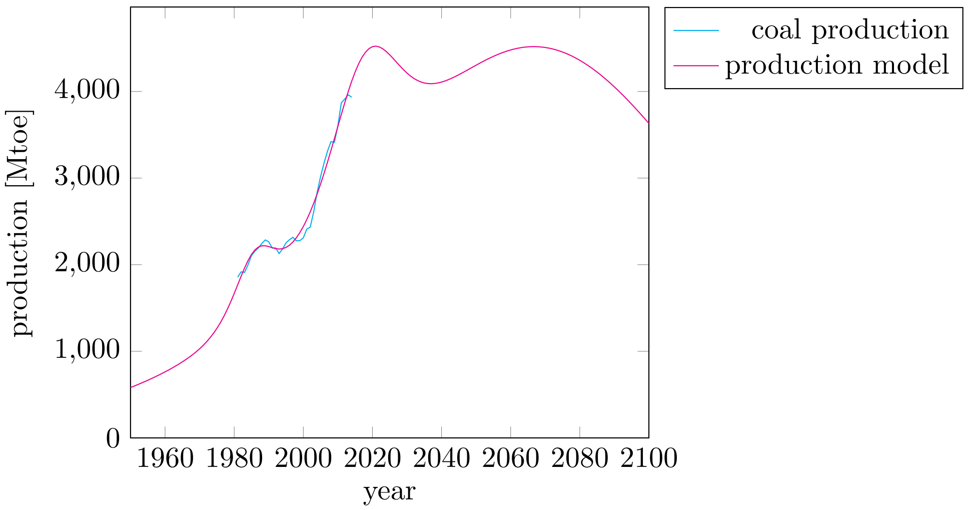


Figure 1.1: Coal gross production

| Fuel | Depletion [GJ] | Upstream emissions [kg $CO_2$e] | Combustion emissions [kg $CO_2$e] | Total emissions [kg $CO_2$e] |
|---|---|---|---|---|
| Coal | 1.167 | 15.93 | 96.21 | 112.14 |

Table 1.3: Emission and depletion factors for coal

### 1.2.2 Oil

Petroleum—or crude oil—is a naturally occurring mixture of generally liquid, but also gaseous and solid, hydrocarbon compounds found in sedimentary rock deposits. It can also contain small quantities of nitrogen, oxygen, and sulfur-containing compounds, as well as trace amounts of metals. The hydrocarbons are mainly alkanes, cycloalkanes, aromatic hydrocarbons and asphaltenes. Crude oil is refined into valuable products, mainly fuels such as gasoline, diesel fuel, or jet fuel, but also lubricating oils, waxes, asphalt and feedstocks for the petrochemical industry.

The process by which petroleum is formed starts with the erosion of rocks by flowing seawater. The eroded particles together with the suspended organic matter settle to sites where the current is less strong. The prominent source of organic matter is marine plankton, but other organisms such as algae and larger marine animals may also contribute. Once settled, the debris is attacked by benthic organisms which transform the organic compounds. Those are then partly transformed by bacteria and buried under the growing cover of sediments. As the pressure increases, the water content diminishes. In this stage, a great part of the carbon is liberated as carbon dioxide, and the remaining is converted into a mixture of new products known as *protopetroleum*.

To form a reservoir, a rock must be porous and permeable, and have an upper trap—usually an impermeable rock. The reservoir rock may or may not be the same rock where the petroleum has formed—the source rock. Anyway, there are two main processes of migration: primary migration is the movement of hydrocarbons from the source rocks to a point where the oil and gas—natural gas—can collect as a continuous phase; secondary migration is the hydrodynamic movement of this continuous phase through the rock, fractures, or faults followed by the accumulation of oil and gas in traps. Once accumulated, gravitational forces cause the oil, gas, and water to segregate, leaving gas in the upper zone, oil in the mid zone and water in the lower zone. In the reservoir, the petroleum may undergo further transformations known as in-situ transformation. Thermal alteration is the action of temperature which cause the heavier fractions of petroleum to crack into lighter ones. Another alteration is deasphalting, or the precipitation of asphaltenes dissolved in light hydrocarbons. Lastly, the action of moving subsurface water may wash the petroleum removing water-soluble compounds and bringing microorganisms which alter the composition of petroleum.

Even though there are natural oil wells, to extract oil it is usually necessary to drill wells into the reservoir. Apart from the primary wells, secondary wells may be drilled as well in which water, steam or other gases are injected to increase the pressure. At first the oil—and gas if present—will naturally flow out due to the reservoir pressure (primary recovery). As the pressure decreases, pumps are used to bring even more oil to the surface (secondary recovery).

The lightest hydrocarbons are gaseous under surface pressure. Alkanes from pentane (5 carbon atoms) to octane (8) are refined into petrol; those from nonane (9) to hexadecane (16) into diesel fuel, kerosene and jet fuel. Heavier fractions of oil produce fuel oil, lubricating oil, paraffin wax and asphalt. To refine oil into more valuable products, there are basically two processes: fractional distillation and cracking. The former consists in exploiting the difference in the boiling point of the various hydrocarbons; the latter in *cracking* heavy hydrocarbons into lighter ones. Most oil products are used as fuels—domestic transportation uses mainly petrol and diesel.

Oil is not evenly distributed through the planet, so it is necessary to deliver it in order to satisfy the global demand. The distribution overseas is mainly done by oil tankers; mainland distribution can be done by pipeline, train, or road. Since oil trade is due to market economy, it is not necessarily distributed to the nearest consumer, so energy losses are greater than necessary.

Conventional oil also includes *natural gas liquids* (NGL) or *wet gas* with high content of liquid hydrocarbons.

### Unconventional oil

Conventional crude oil is that which can be extracted by simple pumping operations. Other types of petroleum, or substances that can yield petroleum-like products, are categorized as unconventional. Unconventional oil includes heavy oil, bitumen, light tight oil (LTO), shale oil, and synthetic crude oil from natural gas (GTL) and from coal (CTL).

Petroleum with a gas-free viscosity between 100–10000 mPa·s and an API gravity[1] of less than 20° is termed *heavy oil*, whereas if its API gravity is less than 10° is may be labelled as *extra heavy oil.* Heavy oil is chemically characterized by its high content in asphaltenes, which makes it have more sulphur and metals than light oil. Heavy oil does not flow if pumped; it has to be stimulated, for instance, injecting steam to decrease its viscosity. That requirement increases the energy expenditure needed to extract it compared to conventional oil. Sometimes the term heavy oil is used as a general term referring both to heavy oils occurring in a reservoir and bitumen.

*Bitumen*, another form of oil tagged as unconventional, is a very viscous—more than 10000 mPa·s—and dense—less than 10°API—form of petroleum. It is found in *tar sands*, also known as oil sands or bituminous sands. Tar sands are sandstone or a porous carbonate rock impregnated with bitumen, which is immobile under reservoir conditions. It is worth noting that, as a consequence, tar sands are mined, rather than pumped. Furthermore, due to the considerable differences in nature between bitumen and conventional oil, specific refining techniques are needed to produce petroleum products. For those reasons, the extraction of bitumen is more costly in terms of both energy and environmental impact.

*Light tight oil* is light oil found in low permeability formations such as tight sandstone or shale. Because of the low permeability of the oil-bearing rock, LTO does not flow as easily as conventional oil. Thus, massive hydraulic fracturing and often horizontal wells are used to extract it. These techniques are not free from controversy, for they allegedly contaminate the underground water surrounding the extraction location. Because LTO is often found in shale formations it is also known as shale oil, but the former term is preferred to avoid confusion with synthetic oil derived from oil shale.

A special class of the previously discussed bituminous rocks is oil shale. Oil shales are fine-grained sedimentary rocks rich in *kerogen*, an organic material reputed to be a precursor of petroleum, that is, immature oil that has not been under the pressure and temperature conditions necessary to form oil. Thus, heating oil shale enough makes it undergo a process called pyrolysis by which the organic material is upgraded to a petroleum-like product known as *shale oil.* Then, shale oil can be refined by conventional methods to yield oil products.

Finally, it is also possible to obtain petroleum products from other resources, such as coal and natural gas. Coal-to-liquids (CTL) and gas-to-liquids (GTL) are several processes that convert coal and natural gas, respectively, to a variety of liquid hydrocarbons that can substitute, or be blended with, petroleum products.

### Production model

The production model of petroleum consists of three curves: two for conventional oil, and another for unconventional oil. The ultimate recovery of conventional oil is $U_{conv} = 2000\,\text{Tb}$, and that of unconventional oil $U_{unc} = 1000\,\text{Tb}$ [**?**]. The parameters of the fitted

[1]API gravity is a measure of the density of petroleum liquids compared to water. An API gravtiy greater than 10° means the liquid is lighter than water.

curves are shown in [TABLE]

Table 1.4: Oil curves' parameters

| Curve | $b$ | $q_{max}$ | $t_m$ |
|---|---|---|---|
| 1 (conventional) | 0.2248 | 9.1537 | 1975 |
| 2 (conventional) | 0.0548 | 25.1520 | 2010 |
| 3 (unconventional) | 0.0552 | 13.7934 | 2047 |

As we can see in the [FIGURE], the models fit the data accurately except maybe in the last years. The reason is that the data available is the production of liquids, and not oil alone. Accordingly, this only has a observable effect in the last years. We will see that the complete model smoothes this difference, which is not significant anyway.

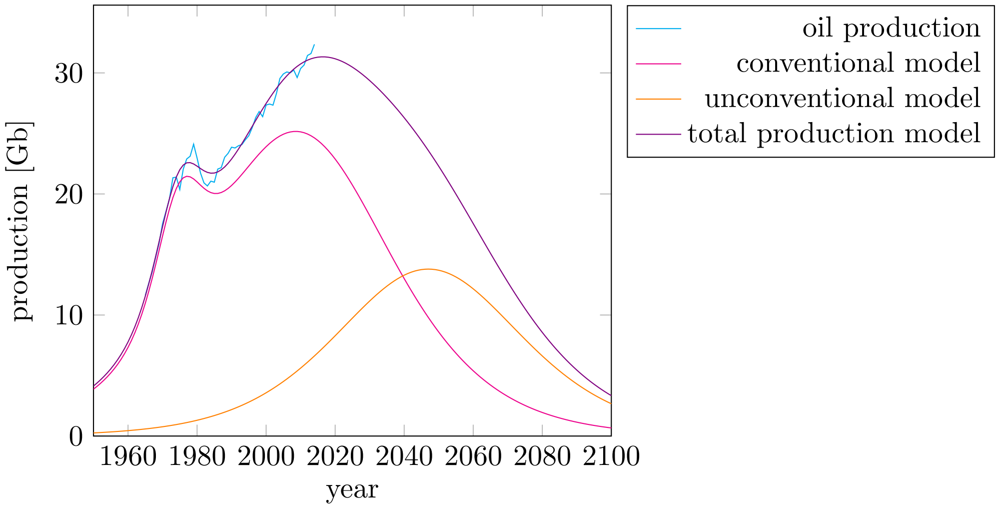


Figure 1.2: Oil gross production

**Oil depletion and emission factors**

Since oil is not consumed directly, the depletion and emission factors will be shown in the energy carriers [SECTION]. The detailed calculations of the depletion of non-renewable resources and upstream emissions derived from the extraction of oil can be found in [APPENDIX].

### 1.2.3 Natural gas

Natural gas is a general term that applies to various gas mixtures commonly *associated* with petroliferous geological formations, although it is also found isolated in reservoirs in which gas is the only occupant and even in coal seams. It consists mainly of methane, but it also may contain higher alkanes up to six carbon atoms, besides other non-hydrocarbon components like carbon dioxide, nitrogen, helium, and hydrogen sulfide. Heavier hydrocarbons and non-hydrocarbons need to be removed for commercial or industrial use of natural gas. The main use of natural gas is electricity generation, but it is also used as a fuel for domestic central heating systems, as a feedstock for the production of fertilisers and several industrial processes, and as a vehicle fuel—*compressed natural gas* (CNG) which can be used in specific or in modified petrol engines.

The origin of natural gas is highly related to that of petroleum. The chemical reactions to form petroleum occur from 130°C, and those to form natural gas—either from already formed oil or directly from its precursor—commence at 180°C. Thus, it may be formed either via a higher temperature catagenesis from protopetroleum and from thermal degradation of petroleum; both processes usually occur parallelly.

The extraction of natural gas is very similar to the extraction of oil, which is not surprising given their close relation. In natural gas reservoirs, the gas can be produced at high pressure; associated, or dissolved, gas must be separated from oil at lower pressures, which increases its cost due to the necessary recompression. Sometimes, it is so costly to recompress the associated gas that is is vented or flared.

Like oil, natural gas is distributed via pipelines in mainland or by ship in large distance overseas as LNG (Liquefied Natural Gas). It is possible for some associated gas fields that its distribution is not economically feasible. In this case, the gas can be flared or injected back into the reservoir to await a possible future market or to increase extraction rates from other wells by repressurising the formation.

### Unconventional gas

*Tight gas* is natural gas produced from reservoir rocks—sandstone or limestone, as conventional gas—that have low permeability. Because of its low permeability, massive hydraulic fracturing —or *fracking*—is necessary to produce at competitive rates.

Similarly, *shale gas* is also found in low porosity rocks, but unlike tight gas, it is found in shale formations. Shale gas has been produced from shales with natural fractures, but recently fracking techniques have been used to extract more gas from shales.

Another type of unconventional gas mistakenly referred to as shale gas is *oil shale gas*, which is synthetic natural gas produced by oil shale pyrolysis. Oil shale gas is the non-condensible fraction of the oil shale products and it is usually treated as a by-product.

*Coalbed methane* is a form of natural gas found in coal seams. The methane is adsorbed in the solid matrix of the coal. To extract it, water needs to be injected through wells drilled into the seam. Coalbed methane contains no hydrogen sulfide —so it is less corrosive than conventional gas—, but it contains more carbon dioxide—so its less energetic. Coalbed methane wells produce at lower rates than conventional gas wells and their initial costs are usually greater.

*Methane clathrates*—or methane hydrates—are solid clathrate compounds in which methane molecules are trapped within a water crystalline structure. It contains up to 160 times the amount of methane per volume than the gas at normal conditions. It is allegedly the vastest resource of fossil fuels, for it is thought that in the ocean floors there are huge amounts of it. However, it has not been proven and the attempts to extract it at economic rates have failed and it is not expected that that will be possible in the foreseeable future.

Another product that could be considered unconventional gas, although it is not methane, is syngas obtained by *underground coal gasification*. The process is the same as described later in the hydrogen [SECTION], but performed underground. This technique allows to reach coal seams that would be otherwise too expensive to mine.

### Production model

The production model of natural gas, unlike the preceding models, is a single generalised Verhulst curve. A generalised Verhulst curve is a generalised logistic curve that includes a parameter of skewness. This curve fitted the data better than the Hubbert curve, even when multiple curves were used. The equation [EQUATION] describes this curve.

$$q(t) = \frac{U\,(2^n - 1)\,e^{\frac{t-t_m}{\tau}}}{n\,\tau\left[1 + (2^n - 1)\,e^{\frac{t-t_m}{\tau}}\right]^{\frac{n+1}{n}}} \tag{1.8}$$

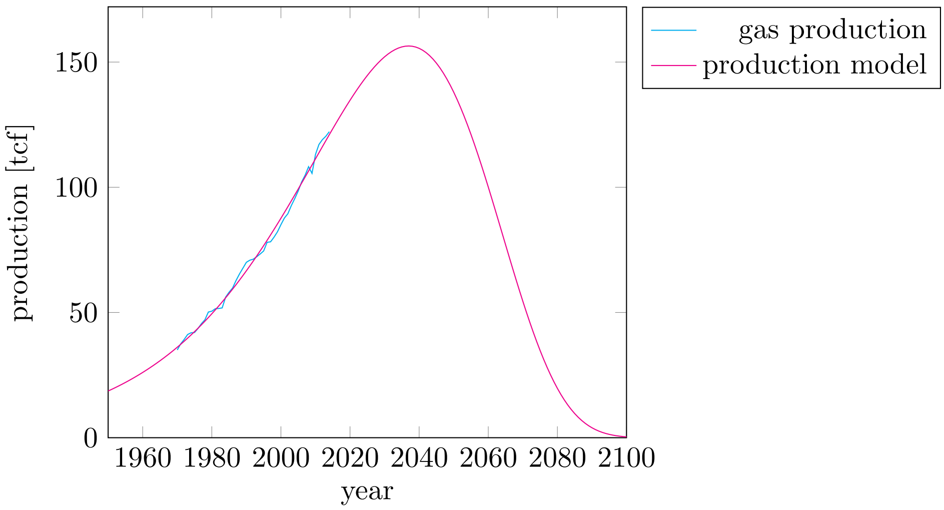


Figure 1.3: Natural gas gross production

With an ultimate recovery of $U = 12000\,\text{Tcf}$ (trillion cubic feet) [**?**] the curve obtained fits the data very well. The parameters of the fitted curve are shown in [TABLE].

### Natural gas depletion and emissions

The calculation of the depletion and emission factors natural gas can be found in [APPENDIX]; the results are listed in table 1.6

Table 1.5: Gas curve's parameters

| Parameter | Value |
|---|---|
| $n$ | $3.007\,10^{-8}$ |
| $\tau$ | 28.22 |
| $t_m$ | 2027 |

Table 1.6: Emission and depletion factors of natural gas

| Fuel | Depletion factor | Upstream emissions [kg $CO_2$e/GJ] | Combustion emissions [kg $CO_2$e/GJ] | Total emissions [kg $CO_2$e/GJ] |
|---|---|---|---|---|
| Natural gas | 1.213 | 31.09 | 55.78 | 86.87 |

### 1.2.4 Nuclear energy

Nuclear power is the main energy source for electricity generation in the UE. Nuclear fuel is different from other fuels, in that the process by which the heat is released is nuclear fission, rather than combustion. Its energy density is much greater than conventional fuels, but the processes to convert the uranium ore into useful fuel and to treat nuclear waste require a lot of energy, too.

Currently, the only natural resource suitable for fission is uranium. Uranium is a radioactive metal. Its more common isotope is U-238 (99.3%), followed by U-235 (0.7%) and U-234 (traces). It occurs naturally in very low concentrations in the Earth's crust—soil, rock, and water—and in uranium-bearing rocks, from where it is extracted.

Unlike fossil fuels, which are more or less readily usable once extracted, uranium has to go through several processes before it can be used. In addition, given its radioactivity, it has to be treated in specialised facilities, and it has to be disposed properly.

#### Reactors and the nuclear fuel cycle

The only fissile uranium isotope is U-235, but it is very rare, compared to U-238. For this reason, uranium has to be enriched to a concentration of around 3–5% of U-235 in order be used in a reactor. However, some of the abundant U-238 atoms are converted into Pu-239—which is fissile—by neutron capture.

There are two main types of nuclear reactors: *thermal* neutrons and *fast* neutrons. Thermal neutrons reactors use a *moderator* to slow down the neutrons emitted in the fission process, where as fast neutrons reactors use no moderator.

There is another major classification of reactors: *burners* and *breeders*. As stated above, uranium-238 can be converted into plutonium-239 by neutron capture. Burner reactors deplete the fissile material—U-235 and the created Pu-239—faster than it is created; breeder reactors create fissile material at a higher rate than it is depleted. Thermal neutrons reactors can only be burners, whereas fast neutrons reactors can be either burner or breeder reactors. All operative power reactors are burner reactors.

In thermal neutrons reactors, the moderator can be heavy water—water which hydrogen is the isotope deuterium—, graphite, or light water. Currently, the vast majority of nuclear reactors are light water reactors (LWR). For this reason, LWR is the reference reactor used in this study, which is based on [**?**].

The fuel cycle is a set of processes the uranium undergoes from the mine to its disposal. A complete picture of the fuel cycle is shown in [FIGURE].The front end of the fuel cycle—from the ore to the reactor—includes the following steps:

**Mining** of the uranium ore—namely uraninite and pitchblende. There are three mining techniques: open-pit mining, underground mining, and in-situ leaching.

**Concentration** of the uranium ore into *yellow cake*, which contains about 75% uranium oxide ($U_3O_8$).

**Refining** and **conversion** into uranium tetrafluoride ($UF_4$).

**Enrichment** of natural uranium to increase its U-235 content to 3–5%.

**Fuel element fabrication**, which consists of the manufacturing of fuel rods that can be used in a reactor.

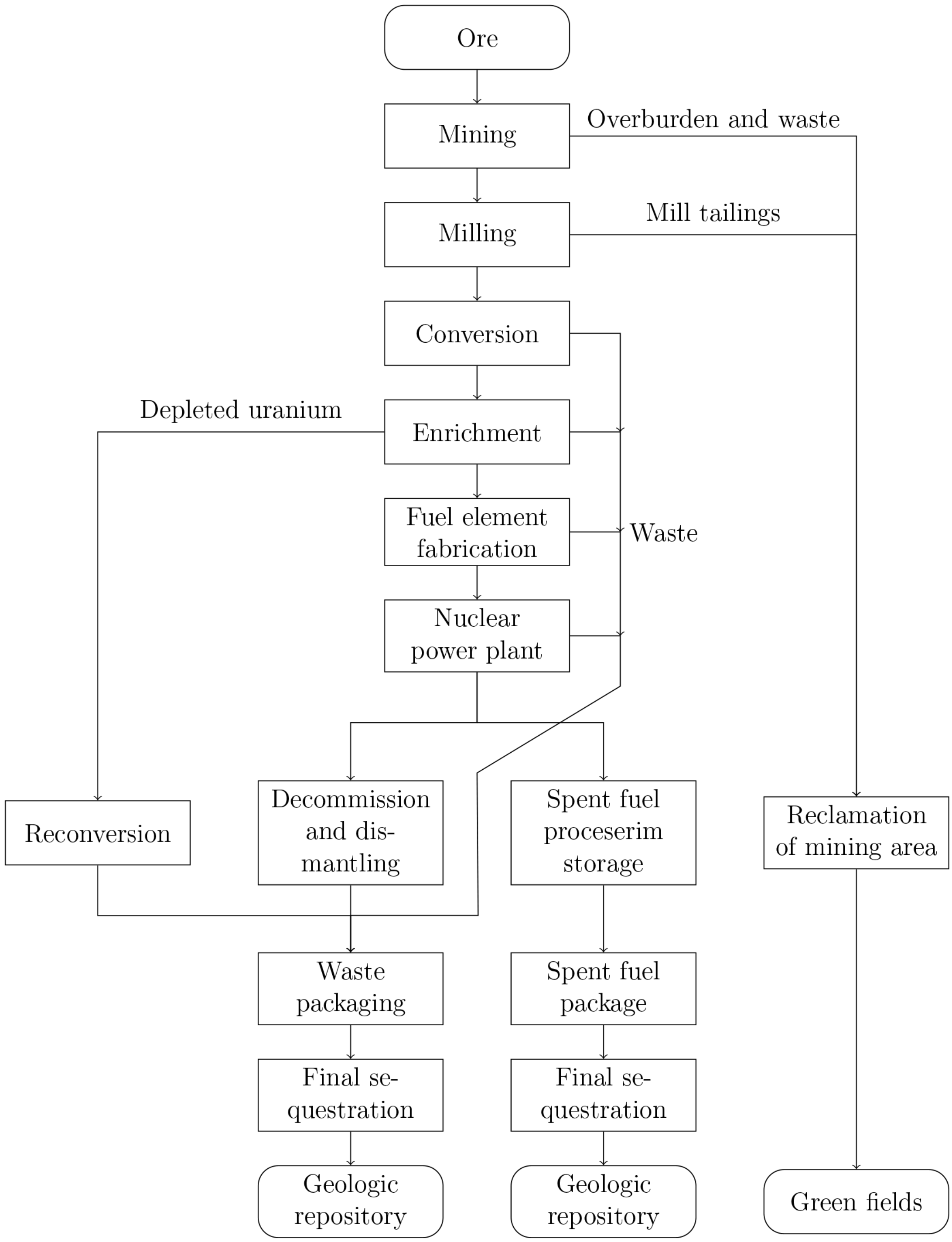


Figure 1.4: Once-through LWR fuel cycle

### Unconventional nuclear energy

Besides the primary uranium sources—i.e. mining—there are secondary sources from which uranium is obtained to fuel nuclear power plants. Secondary uranium sources include the reprocessing of spent fuel, the re-enrichment of depleted tails, and the civilian and military stocks—weapon-grade highly enriched uranium (HEU) and warheads. It is curious that, as shown in [FIGURE] the cumulative difference between supply and demand of uranium follows the same curve as the number of nuclear warheads. What can be deduced from that figure is that most of secondary uranium sources come from stocks. In fact, in 2002, more than half of the uranium used in power generation came from dismantled nuclear weapons. In the particular case of the two most *nuclearised* nations of the world—the US and Russia—, in 2013 the *Megatons to Megawatts Program* was completed [?]. This program was an agreement between the US and the Russian Federation. Under this program, the latter agreed to supply low-enriched uranium from military-grade HEU to the former.

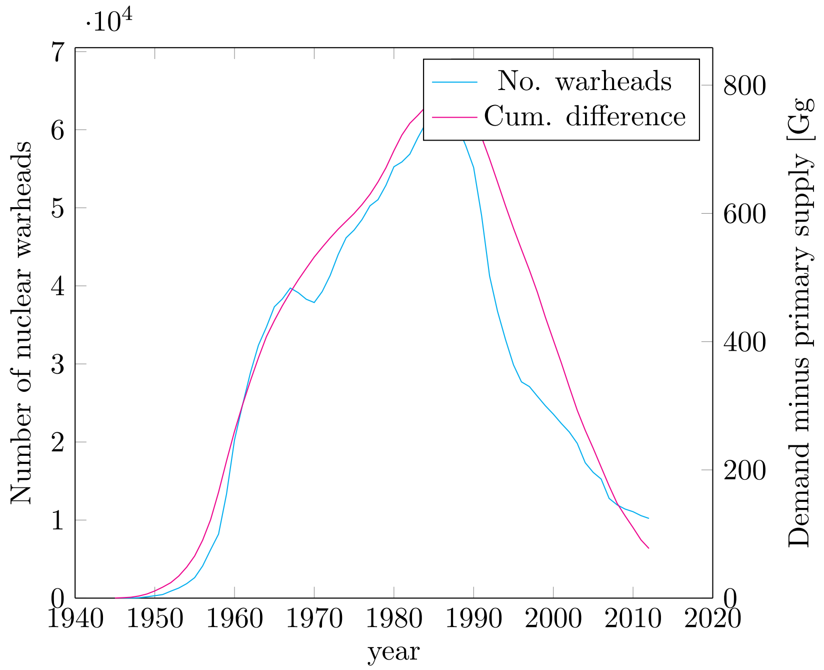


Figure 1.5: Nuclear warheads and cumulative difference between demand and primary supply

Other forms of nuclear energy, tagged as *unconventional nuclear energy* include the uranium from seawater, fast breeder reactors, thorium as a nuclear fuel, and fusion energy. These technologies are unlikely to be mature and profitable in the short-term, if ever, so it is not convenient to make predictions based on the supposition that they will be available. Therefore, the forecasts used here assume that the current technology alone will be available in the short-term.

### Production model

The production model of uranium consist of six Verhulst curves. It should not surprise anyone, because nuclear energy has been a matter of politics since its advent. As it happens, the supply–demand gap is caused by politics rather than by market dynamics. The parameters of the curves are shown in [TABLE].

Table 1.7: Uranium curves' parameters

| Curve | $U$ | $n$ | $\tau$ | $t_m$ |
|---|---|---|---|---|
| 1 | 290.55 | 1.45 | 1.800 | 1960 |
| 0 | 69.22 | 7.53 | 0.67 | 1998 |
| 3 | 1225.12 | 3.101 | 5.77 | 1980 |
| 4 | 227.51 | 0.47 | 2.46 | 1987 |
| 5 | 196.49 | 1.85 | 1.44 | 1981 |
| 6 | 4425.729 | 0.22 | 10.54 | 2029 |

The resulting curve can be seen in [FIGURE].

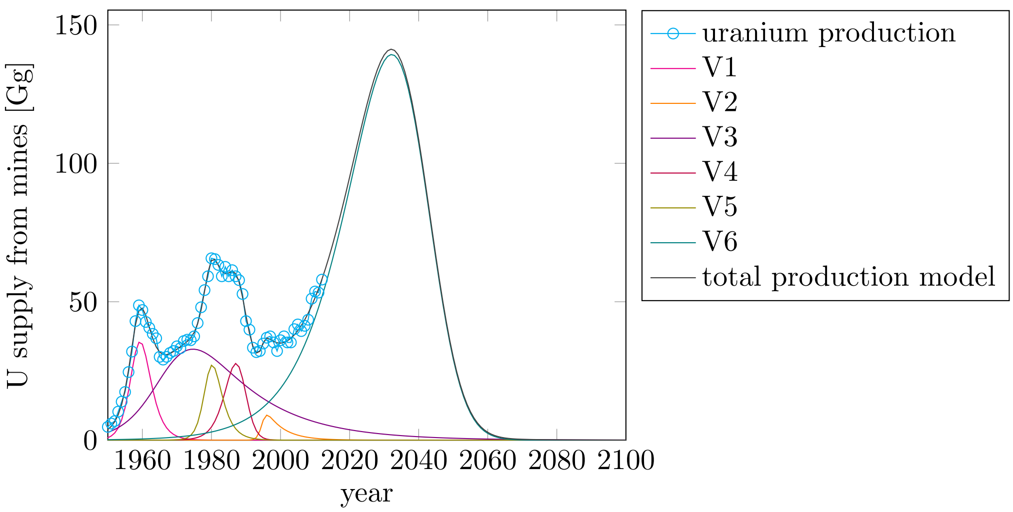


Figure 1.6: Uranium production

### Uranium depletion and emissions

Since uranium is not used directly, but rather as a means to obtain electricity, the depletion and emission factors given (see [TABLE]) refer to electricity from nuclear origin, not uranium consumed itself—it has not a LHV. Therefore, these values should be looked at carefully, and not compared directly with fossil fuels, for instance, because they have the energy conversion efficiency included in them.

| Fuel | Depletion factor | Emission factor [kg $CO_2e$/GJ] |
|---|---|---|
| Uranium | 1.186 | 13.83 |

Table 1.8: Emission and depletion factors of uranium (electricity consumed)

The calculations can be found in the [APPENDIX]. It should be noted that, just as fossil fuels' figures do not include the global warming effects, the uranium numbers do not take into account the energy costs associated with nuclear disasters —such as Chernobyl or the more recent in Fukushima—. In addition, the possible energy shortages may make the maintenance of nuclear plants more difficult, making accidents more probable and the long life of nuclear residues make them more prone to natural disasters such as earthquakes. However, since there is no way to model that, we will assume that the ratio of accidents will remain constant, and that the cost of them is not included in the life cycle analysis.

### 1.2.5 Hydro, solar and wind energy

When we speak about renewable energy sources, perhaps the ones that come to mind first are hydro, wind and solar power. In a human timescale, they are indeed inexhaustible; as long as the Sun shines, there will be sunlight—evidently—, wind, and the water cycle will go on. However, to benefit from them, some infrastructure is needed. Dams, in the case of hydropower, windmills for capturing wind power and solar panels to put solar radiation to use. Those are currently built using fossil energy, so when we use *renewable* energy we are consuming fossil energy indirectly.

| Energy source | Depletion factor | Emission factor [kg $CO_2e$/GJ] |
|---|---|---|
| Hydro | 0.011 | 0.85 |
| Wind | 0.053 | 3.97 |
| Solar (PV) | 0.107 | 7.93 |
| Solar (Th) | 0.548 | 40.79 |

Table 1.9: Hydro, wind and solar depletion and emission factors [APPENDIX]

### Hydro

Hydraulic energy is the gravitational potential energy of water. It is actually an almost direct form of solar energy: hydropower exploits the energy contained in water due to the water cycle, which is fueled by Sun radiation. To exploit that energy efficiently, dams are constructed on rivers in order to increase the height of the head and to be able to regulate the flow of water. A hydraulic turbine transforms the kinetic energy of water into rotational kinetic energy, which is converted to electricity by a generator.

Hydraulic power is very cheap, in terms of energy investment, and countries with huge amounts of water resources, such as Norway or Brazil, already produce the best part of their electricity by means of hydraulic power stations. It is no surprise, then, that the growing potential of hydropower is very limited. [OLIVARES] puts this limit to 1 TW of electricity production, of which almost a half is already being produced.

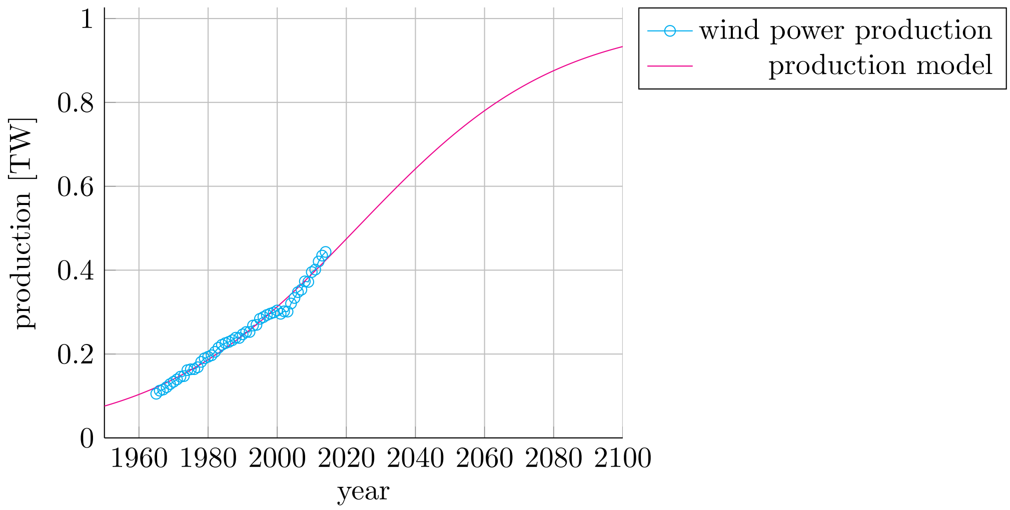


Figure 1.7: Hydropower production

### Wind

Wind is the movement of the atmospheric air. The two principal driving forces are the uneven heating of the atmosphere—which causes differences in the atmospheric pressure—, and the rotation of the planet. It has been suggested that the condensation and evaporation of water are also major factors driving atmospheric dynamics [MAKARIEVA].

Wind power is the use of the kinetic energy of the wind, which is extracted by means of turbines, usually to produce electricity. The wind kinetic energy flowing through an area $A$ during the time $t$ is given by the [EQUATION]. However, the theoretical maximum efficiency any wind turbine can achieve, regardless of its design, is indicated by the Betz's law, and it has a value of 59.3%. In practice, this value is reduced even further; actual wind turbines can reach efficiency values around 80% of the Betz limit.

$$E = \frac{1}{2} A\rho v^3 t \tag{1.9}$$

Windmills can be constructed onshore or offshore. Generally, offshore wind is steadier and stronger than in land, but the corrosion caused by seawater and the technological challenge that constructing windmills several kilometres away from shore poses, make onshore wind farms more profitable. While there is a physical limit of how much energy can be extracted from the wind, the major deterrents are the material requirements of the infrastructure needed. The average power that can be extracted in small wind farms is 4–7 $W/m^2$, but in large farms—several hundreds of square km—this value decreases to 1 $W/m^2$ [CRASHOIL,OLIVARES].

Olivares [OLIVARES] depicts three possible scenarios of future explotation of wind power. The low occupation of continental shelfs and mainland surface scenario is enough to produce 8.6 TW of electric power with a wise explotation of copper, nickel, lithium, and platinum reserves. With a capacity factor of 0.31 [OLIVARES], it is necessary 27.74 TW of installed capacity, which will be reached following a logistic function.

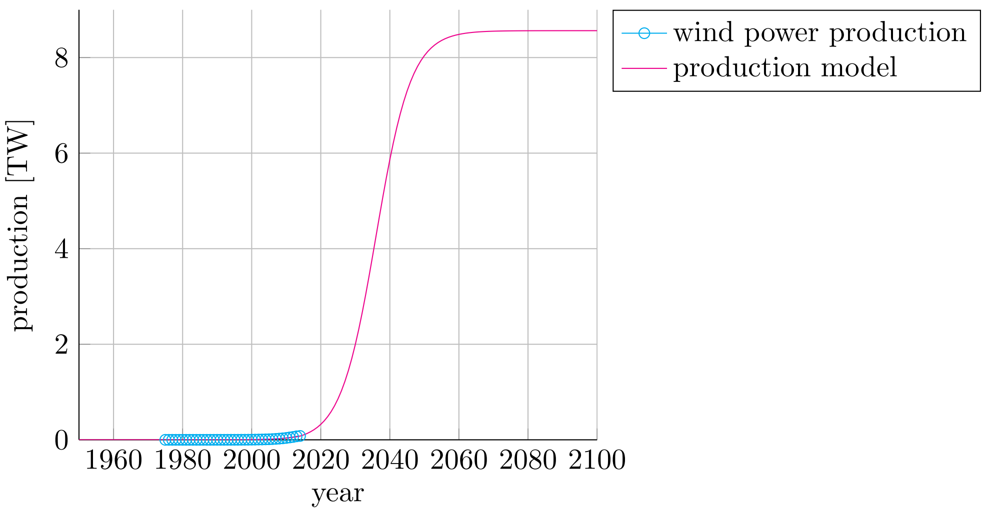


Figure 1.8: Wind power production

### Solar

Finally, solar power is the most direct way to benefit from the Sun. There are mainly two forms of solar power. First, there is thermal solar power. Solar panels gather solar radiation in the form of heat, which can be used directly as a source of heat or be converted into electricity. Second, photovoltaic solar power. Photovoltaic panels turn solar radiation directly into electricity making use of the photoelectric effect. For the purpose of producing electricity, photovoltaic panels are more efficient.

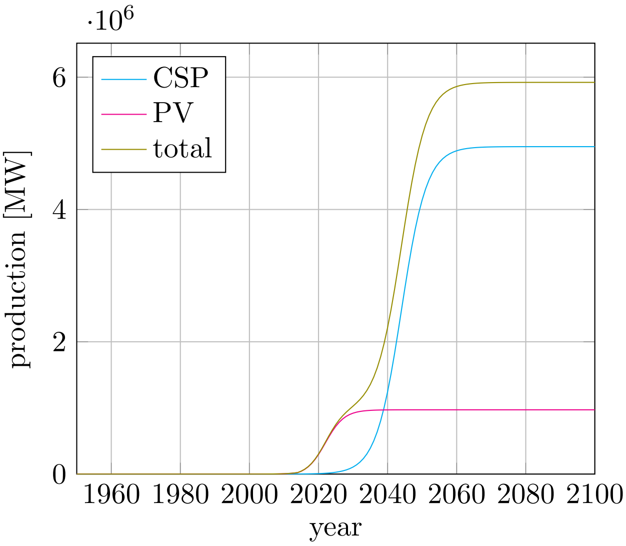


Figure 1.9: Solar power production

### 1.2.6 Geothermal power

Geothermal energy is the thermal energy generated and stored in the Earth. The Earth has three different layers at different temperatures:

> **The core**, which is solid inside and liquid outside, can reach temperatures up to 4200°C.
>
> **The mantle**, with temperatures from 3000°C to 1000°C. It is plastic towards the centre and solid towards the surface.
>
> **The crust** is the outer shell of the planet. Its temperature ranges from 1000°C in the contact with the mantle, to 15–20°C on the surface.

The result of this distribution is that 99% of the Earth's mass is at more than 1000°C. Therefore, the difference of temperature make the heat flow outwards. The origin of this heat can be attributed to three factors:

> **Radioactive decay** of the isotopes presents in the crust and mantle, mainly U-235, U-238, Th-282, and K-40.
>
> **Initial heat** liberated when the planet formed, which is still reaching the surface.
>
> **Core crystallisation**. The outer core, which is liquid, is continually crystallising, releasing heat in the transition zone between the inner and outer core.

Olivares [**?**] puts the limit to geothermal power production to 0.5 TW. With a capacity factor of 0.7 [**?**], fitting the data of geothermal power capacity [**?**] to a logistic curve results in the evolution of geothermal power production shown in [FIGURE].

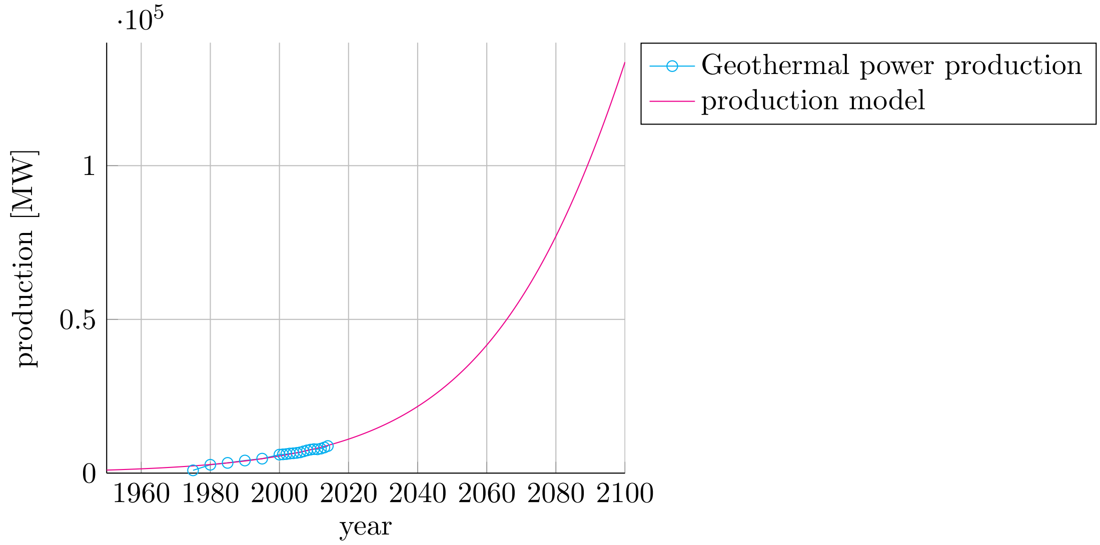


Figure 1.10: Geothermal power production

### 1.2.7 Biomass and waste

Biomass is a renewable source of energy. However, the burden put upon biofuels as substitutes of fossil fuels in transport applications might not be justified. Olivares [?] that the limit of biofuels production is 1 TW. The energy from biomass obtained at small scale—for instance, wood collected locally as a fuel for heating homes—cannot be considered a primary energy source, so it is not included here. Fitting the data [?] into a logistic curve with the limit just mentioned manifests that [FIGURE], even though we are far from that limit, it will not be sufficient to substitute petrol or diesel alone.

Waste—or, more precisely, Municipal Solid Waste (MSW)—, on the other hand, is a source of energy obtained by burning the waste generated by human activity. It is not a renewable energy source and, even though it relieves landfills from overfilling and provides energy, it is not a clean energy solution. For this reason, and the fact that generated waste depends on goods produced—and those are not in the scope of this thesis—, MSW will not be included in the analysis of the global energy model.

### 1.2.8 Global model

Adding up all the previous models, results in a global energy supply shown in [FIGURE].

However, all of this energy is not the energy available, because producing energy consumes energy. As seen on the [SECTION], the measure of the energetic cost of energy is the EROI.

Using the EROI values of the [TABLE], the resulting supply of available energy is that of [FIGURE].

This numbers, though, are lacking an essential piece of information: this energy has to be split distributed over the whole population. The population, obviously, is not

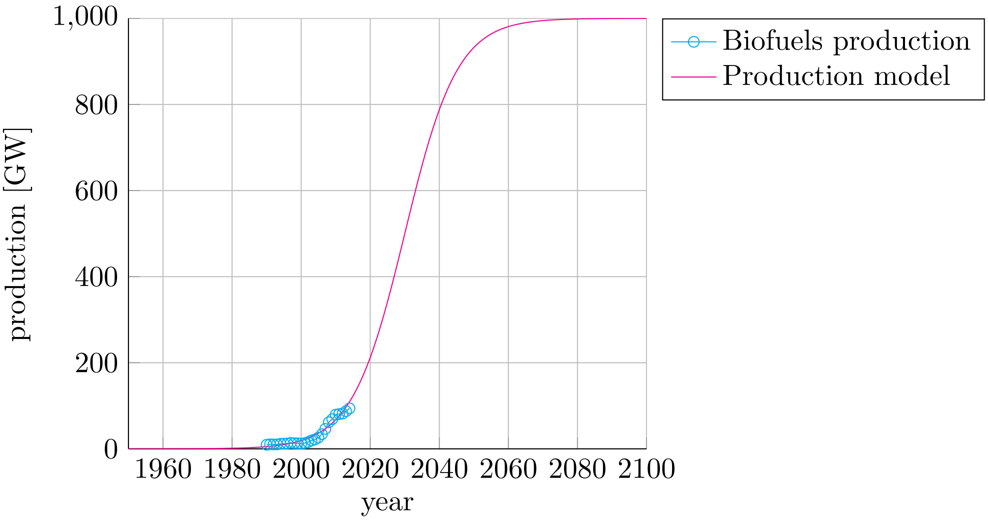


Figure 1.11: Biofuels production

constant over time. The United Nations presents four possible scenarios of population growth, depicted in [FIGURE]. For our analysis, we will use the *medium fertility* scenario, as it represents a compromise between the different options.

It should be borne in mind that resources are not distributed equally over the population. Since it is not the intention of the author to assume that this fact will remain true in the future, two scenarios are contemplated. In the first scenario (*utopian*) the energy is distributed evenly across the population; in the second scenario (*pareto*) the energy is distributed according the Pareto Principle—that is, the 80% of the energy is consumed by the 20% of the population. In this second scenario, it is assumed that the user of the vehicle to be designed is part of the 20% and that inside the rich group the energy is evenly distributed.

Because we are considering transport energy, we will assume that the ratio of the energy used by transport, which is about one fifth [?], is constant over time. The time span studied is 2020–2040. Both the energy and population are integrated over time to obtain an average over the time span.

The results are listed in [TABLE]

Table 1.10: Distribution of energy across the population

| Scenario | Energy (2020–2040) [PJ] | Population (2020–2040) [billions[1]] | Power per capita [W] | Transport power per capita [W] |
|---|---|---|---|---|
| *Utopian* | 215.31 | 159.18 | 42.89 | 8.58 |
| *Pareto* | 172.25 | 31.84 | 171.57 | 34.31 |

[1] 1 billion = $10^9$

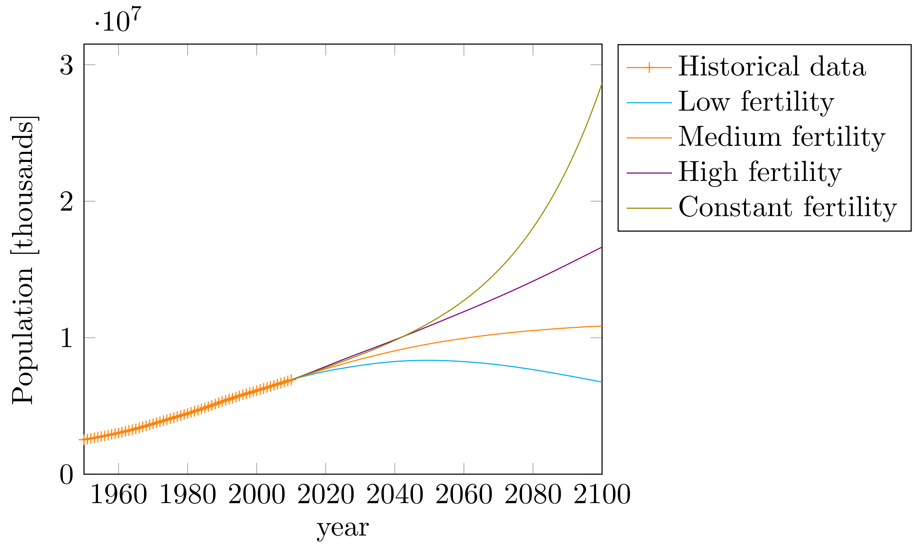


Figure 1.12: World's population evolution

## 1.3 Fuels and energy carriers

Energy carriers are forms or systems of energy that are used to produce work, heat, or to operate chemical or physical processes. They are different from energy sources in that are part of the middle stages of the energy system. Whilst primary energy sources are found in nature as they are, energy carriers are produced by either primary energy sources or other energy carriers. In regard of transport, they are mainly fuels and electricity. In what follows, four energy carriers are described, and their respective depletion and emission factors are calculated.

### 1.3.1 Petrol

Petrol—or gasoline—is a fuel obtained from petroleum. Together with diesel oil, it is the most used fuel for cars. Diesel engines tend to be more energy efficient, and vehicles using it emit less $CO_2$ than its petrol counterparts. However, the combustion of diesel fuel in vehicles produce much more particulate matter, sulphur oxide and nitrogen oxides. For that reason, some cities—such as Barcelona [?], Paris , or London [?]—are restricting the access of Diesel vehicles. And for that reason too, only petrol is analysed here as a possible fuel for urban vehicles.

The depletion factor

### 1.3.2 Electricity

Electricity is the *universal* energy carrier. It is produced from heat—thermal power stations—, mechanical energy—hydropower, wind energy, wave energy, etc.—, or directly from light—photovoltaic solar power. It is, however, difficult to store compared to fuels. Even so, electricity use is increasing owing to, mainly, two factors: virtually all types of renewable energy produce electricity, and it does not emit pollutants where it is being consumed. The depletion and emission factors of electricity, as produced in the period 2020–2040, are those of [TABLE] (see [APPENDIX]).

Table 1.11: Depletion and emission factors of electricity

| | Depletion factor | Emission factor [kg $CO_2$e/GJ] |
|---|---|---|
| Electricity | 2.225 | 161.40 |

### 1.3.3 Biofuels

Biofuels are fuels produced from biomass through biological processes. It is a wide category that includes bioalcohols (ethanol, methanol, butanol), biodiesels, biogas (methane), syngas and even solid fuels. In the field of liquid fuels for transport, only bioethanol and biodiesel are mature technologies, but we have only considered bioethanol since it can run on unmodified or slightly modified petrol engines—Diesel engines are not contemplated here—and also serves as feedstock for producing hydrogen.

The use of biofuels instead of fossil fuels presents numerous advantages, the more evident being that it is a renewable resource. In addition, they help reduce the carbon footprint of transport, for the carbon content of biofuels comes from atmospheric $CO_2$.

However, there are several drawbacks too. First, the production of biofuels currently consumes fossil energy and therefore emits greenhouse gases into the atmosphere. Another major concern is land and water use, which are limited resources; consequently, biofuel production compete with food production making the latter more expensive.

#### Bioethanol

Ethanol is already produced in large scale. Hydrous ethanol is the most concentrated grade that can be obtained by simple distillation. Its concentration is up to 96% of ethanol and 4% water. It can be used as neat ethanol or blended with petrol in any proportion in flexible-fuel vehicles (FFV). Anhydrous ethanol is obtained by dehydrating hydrous ethanol and has a purity of at least 99%. It can be blended with petrol in proportions up to 24% to be used in regular petrol engines. The two main producers of bioethanol are Brazil—from sugarcane—and the U.S.—from corn.

#### Sugarcane ethanol

The process starts with crushing the cane to obtain the juice and bagasse. On the one hand, bagasse is used as fuel for the mills, which are based on cogeneration steam cycles; these are capable to provide the mills' energy demand plus bagasse and electricity surplus. On the other hand, the juice follows to fermentation, producing the wine, which is then distilled to obtain hydrous ethanol. If the desired product is anhydrous ethanol, a further dehydration process is needed.

The main residues are filtercake mud and stillage, which are used as fertilisers. That helps reducing the need for mineral fertilisers and therefore reduce the energy consumption of the agricultural phase.

| | 2005/2006 | 2020 |
|---|---|---|
| Energy (MJ/t cane) | | |
| Fossil input | 233.8 | 262.0 |
| Ethanol | 1926.4 | 2060.3 |
| Bagasse surplus | 176.0 | 0.0 |
| Electricity surplus | 82.8 | 972.0 |
| $r_E$ | | |
| Ethanol | 8.2 | 7.9 |
| Ethanol+bagasse | 9.0 | 7.9 |
| Ethanol+bagasse+electricity | 9.3 | 11.6 |

Table 1.12: Renewable output to fossil input ratio of sugarcane ethanol

In the renewable energy sector the renewable output to fossil input ratio ($r_E$) is widely used to compare the sustainability of energy sources. The values for sugarcane ethanol in Brazil are listed in table 1.12. Assuming all fossil energy consumed is diesel fuel, the depletion factor of ethanol is

$$d_{ethanol} = \frac{d_{diesel}}{r_E} = \tag{1.10}$$

The GHG emissions in the production of ethanol are, basically, cane trash burning emissions, agricultural inputs and transport emissions. The photosynthesis cycle is excluded since the carbon fixed by the plant is emitted by burning cane trash, bagasse, ethanol and during fermentation. Total life cycle emission factor for ethanol are 18.5 and 14.6 kg $CO_2$e/GJ in the 2005/2006 and 2020 scenarios, respectively.

The production of ethanol is done to obtain ethanol; bagasse and electricity surpluses are co-products. Since the aim of this study is to compare different fuels for transport, energy inputs and emissions must be allocated to ethanol alone. Thus, the depletion and emission factors for sugarcane are those of 1.13

| Fuel | Depletion [GJ] | Upstream emissions [kg $CO_2$e] | Combustion emissions [kg $CO_2$e] | Total emissions [kg $CO_2$e] |
|---|---|---|---|---|
| Sugarcane ethanol | 0.166 | 14.6 | 0 | 14.6 |
| Corn ethanol (combined) | 1.087 | 48 | 0 | 48 |

Table 1.13: Emission and depletion factors per GJ of bioethanol consumed

#### Corn ethanol

Corn ethanol is made from corn kernels. A more accurate term would be starch ethanol, since corn grains include large amounts of starch, which is easily fermented to create ethanol. In fact, ethanol can be manufactured by the fermentation of any starch or sugar-producing plant—like sugarcane. However, in the U.S. almost all starch ethanol is made from corn, hence its name.

The process is very similar to that of sugarcane ethanol: corn kernels are crushed, then the resulting juice is fermented and, finally, the wine is distilled. Still, the production of ethanol from corn is not as profitable as from sugarcane. The energy balance of corn ethanol production is listed in 1.14. Again, the energy inputs have been completely allocated to ethanol.

| Feedstock | Energy input [MJ/L] | $r_E$ |
|---|---|---|
| Grain | 22.4 | 1.05 |
| Stover | 5.8 | 4.02 |
| Combined | 19.2 | 1.21 |

Table 1.14: Energy balance for corn ethanol (starch, cellulosic and combined)

Another pathway to obtain ethanol from corn is from its shell. Cellulosic ethanol is obtained from lignocellulose—cellulose, hemicellulose and lignin—which is the structural material present in corn stover and virtually every plant. The process of fermenting cellulose is much more complex that the process of fermenting starch. First, an acid must be added to unweave the three components, and then break hemicellulose into four sugars. In the meanwhile, cellulose is freed and needs to be broken into glucose by enzymes. Finally, the five sugars must be fermented, which is more difficult than fermenting only one sugar.

Since the agricultural phase is shared with starch ethanol production, it does not need to be included in the energy balance of this process (see 1.14). If starch and cellulosic ethanol is to be obtained from the same plantation, there is an important limiting factor that has to be noted: corn stover is used by farmers to prevent soil erosion and degradation, so not all of it can be used to make ethanol. The combined energy balance is found in 1.14 (for details, see [APPENDIX]).

### 1.3.4 Hydrogen

Hydrogen is a very promising fuel. It has a lower heating value in mass about three time that of petrol, and can be used in fuel cells or even in internal combustion engines. It is abundant—it comprises nearly 90% of all matter in the Universe—, but pure hydrogen is very rare in nature. As a consequence, some process has to be made in order to obtain it. In the next lines several processes concerning the obtention of hydrogen are described.

### Biomass gasification

Hydrogen gas can be obtained from biomass. It is done mainly by first obtaining methane in bioreactors and then following the same process as natural gas reforming.

### Coal gasification

Coal is a good fuel for thermal power stations: it is consumed nearly as it is extracted and it is easy to transport. But when it comes to fuels for transport, it is a very poor option. However, hydrogen may be obtained from it.

$$3\,C + O_2 + H_2O \longrightarrow H_2 + 3\,CO \tag{1.11}$$

The reaction [EQUATION] produces syngas—a mix of hydrogen and carbon monoxide. This reaction is endothermic, but the heat needed is usually obtained through exothermic reactions in the gasifier itself. The process can be made in-situ within coal seams—underground coal gasification—or in coal refineries. If the desired product are alkanes, the syngas is conducted to a Fischer-Tropsch reactor; if the desired product is hydrogen, the gas must undergo a further process, known as water–gas shift reaction [EQUATION].

$$CO + H_2O \longrightarrow CO_2 + H_2 \tag{1.12}$$

Even though this process is called coal gasification, the desired gas—hydrogen—comes from the water. The main component of coal—carbon—is used to *capture* the oxygen from water, thus freeing hydrogen, but also carbon dioxide. However, this downside can be mitigated capturing the $CO_2$, at the expense of more energy being consumed.

Without carbon capturing, the process has a surplus of electricity—obtained from the residual heat—. However, and as explained before, all energy consumed and emissions are allocated to hydrogen. With carbon capturing, the process requires more electricity than it is generated.

### Natural gas reforming

Natural gas is a similar fuel to hydrogen in that it is a gas. However, natural gas can only be burned, whereas hydrogen can be burned and as feedstock for fuel cells, hence the interest in this process. The steam–methane reforming process is as follows:

$$CH_4 + H_2O \longrightarrow CO + 3\,H_2 \tag{1.13}$$

Again, a further water–gas shift reaction is needed to obtain purer hydrogen. The steam–methane reaction is strongly endothermic; the water–gas shift reaction is mildly exothermic. Therefore, the overall process requires energy, namely natural gas itself and electricity. If the carbon dioxide is to be captured, even more electricity is needed.

**Ethanol reforming**

Ethanol can also be fed into a steam-reformer to yield hydrogen. The reaction is rather complex, giving intermediate hydrocarbons, but the overall reaction is

$$C_2H_5OH + 3\,H_2O \longrightarrow 2\,CO_2 + 6\,H_2 \tag{1.14}$$

This reaction is endothermic as well and produces carbon dioxide. However, if the feedstock is bioethanol, the $CO_2$ emitted has already been taken into account in the production of ethanol. Thus, the emissions of this process are not counted.

**Water electrolysis**

Water is composed of hydrogen and oxygen; thus, splitting water molecules yields hydrogen and oxygen. This simple process is called electrolysis, because it is done by electricity. The advantage of this process is that it is very straightforward and only requires electricity, though if heated, water molecules are more easily broken. Plus, if electricity is obtained from clean sources, net emissions are zero.

$$2\,H_2O \longrightarrow 2\,H_2 + O_2 \tag{1.15}$$

| Process | Depletion factor | Emission factor [kg $CO_2$e/GJ] |
|---|---|---|
| Coal gasification | 2.087 | 191.21 |
| Coal gasification CCS | 2.226 | 53.60 |
| Natural gas reforming | 1.703 | 122.62 |
| Natural gas reforming CCS | 1.748 | 56.94 |
| Ethanol reforming (corn) | 1.303 | 96.94 |
| Water electrolysis | 3.618 | 262.46 |

Table 1.15: Emission and depletion factors for hydrogen

## 1.4 Materials

On the subject of energy, material resources are as critical as the energy resources themselves. Some energy sources or forms of making use of energy require scarce materials. As a consequence, its use must be assessed in order to evaluate its sustainability. However, assessing the sustainability of certain materials proves very difficult. First, there is no direct equivalence between materials that can be used for the same purpose. We can compare solar power to wind power, but comparing lead and lithium is not so straightforward, since those two materials are used for other purposes other than for making batteries. Furthermore, materials can be recycled, whereas energy cannot. Thus, material depletion is not included in the analysis of sustainability. Despite that, the energy required to extract and transform materials into commodities is taken into account.

In table [TABLE] a representative list of all the materials used in a vehicle is presented, as well as the energy required to produce them and the emissions associated to their production. In the following lines, the materials which information have not been directly extracted from the literature, or require special attention due to its unusualness, are further discussed.

### Platinum

As shown in table [TABLE], the energy requirements of platinum is disproportionately higher than the rest of metals. The reason is that platinum occurs in nature along with other metals [?]. Therefore, the energy required to extract platinum is shared with those other metals. If the energy is allocated by mass produced, the energy value is substantially lower than the figure presented. However, platinum is a precious metal and its price is much higher than the others. Consequently, price allocation is a more realistic approach, since those metals, from an economic point of view, are co-products of the extraction of platinum.

### Carbon fiber

From [?], we know the energy requirements and emissions related to the production of carbon fiber. Knowing that carbon fiber represents 50% of the mass of carbon fiber reinforces polymer—the other half is epoxy resin—, and that for each unit of mass of CFRP 1.14 units of mass of the mentioned materials are needed [?], we obtain the values presented in [TABLE].

### Glass

First, from the data of float glass production figures [?], we obtain the ratio of emissions to energy consumption of glass production. Then, from [?], we know that the mass of the windshield represents 39% of the total mass of glass in the car. Windshields are composed of two layers of float glass, and a layer of plastic—usually PVB—that lies in between. Also, the same document provides the energy requirements of the windshield and other glasses. With that information we can calculate the total energy requirement. With the ratio of emissions to energy consumption of glass production we can estimate the emissions. The results are those of [TABLE].

### Paint

The data of energy requirements and GHG emissions of the production of paint are taken from [?]. Those numbers are for a whole vehicle. In the same document, it is stated that the vehicle analysed is a SUV, which is assumed that has a mass of 2000 kg, and the mass of the paint represents 1.3% of the total mass of the vehicle. Using those numbers, the result is the value shown in [TABLE].

### Elastomers

The elastomers—used mainly in tyres—can be either synthetic (SBR) or natural. Synthetic rubber represent 57% of the total of the rubber used [**?**]. With the energy requirements and GHG emissions of each type of rubber, the weighted average can be computed.

### Vehicle fluids

Vehicle fluids include brake fluid, engine oil, engine/powertrain coolant, transmission fluid, and windshield fluid. Steering fluid is not included because it is assumed that the vehicles analysed use electrical power steering. From [**?**], we get the energy requirements and the emissions associated to each fluid—the emissions are given desegregated, of each greenhouse gas—. Also, the number of lifetime replacements (see [TABLE]) are given in the same reference.

Multiplying the energy and emission figures by the number of replacements results in the values listed in [TABLE].

Table 1.16: Energy requirements and emissions of material production

| Type | Material | Energy [MJ/kg] | GHG emissions [kg $CO_2$e/kg] |
|---|---|---|---|
| Metals[?] | Aluminium (cast) | 121.7 | 9.86 |
| | Aluminium (wrought) | 174.0 | 14.18 |
| | Copper | 45.7 | 3.03 |
| | Iron | 35.0 | 2.43 |
| | Magnesium | 397.0 | 28.93 |
| | Nickel | 191.2 | 13.83 |
| | Platinum | 223393.1 | 18767.03 |
| | Steel (average) | 53.5 | 4.06 |
| | Zinc metal | 46.0 | 1.75 |
| | Zinc oxide | 84.0 | 10.95 |
| Plastics[?] | ABS | 102.0 | 3.91 |
| | Nylon (average) | 102.0 | 3.91 |
| | Nylon 6 | 110.9 | 8.97 |
| | Nylon 66 | 122.0 | 6.66 |
| | Other | 122.0 | 6.66 |
| | Other resins | 109.6 | 4.95 |
| | PC | 104.9 | 5.02 |
| | PET | 71.2 | 3.12 |
| | Polyvinyl Butyral | 71.2 | 3.12 |
| | PP | 80.8 | 2.41 |
| | PUR (average) | 76.0 | 2.77 |
| | PUR flexible | 72.5 | 3.36 |
| | PUR rigid | 67.8 | 2.98 |
| | Plastic (average) | 89.8 | 3.63 |
| Composites | Carbon fiber (CFRP) | 433.7 | 28.27 |
| | Glass fiber (GFRP)[2] | 88.0 | 10.80 |
| Others | Elastomers | 82.1 | 4.23 |
| | Fabrics[?] | 115.5 | 13.32 |
| | Friction material[?] | 433.7 | 28.27 |
| | Glass | 76.0 | 6.49 |
| | Paint | 51.1 | 1.62 |
| | Carbon paper[?] | 2133.0 | 170.00 |
| | Nafion[?] | 22.0 | 0.32 |
| | PTFE[?] | 114.0 | 10.52 |

Table 1.17: Lifetime replacements of the fluids

| Fluid | Lifetime replacements |
| --- | --- |
| Brake fluid | 3 |
| Engine oil | 39 |
| Engine/powertrain coolant | 3 |
| Transmission fluid | 1 |
| Windshield fluid | 19 |

# Chapter 2

# Transport in the city of Barcelona

Transport is one of the biggest sectors of the world's economy. As such, this industry is also one of the biggest energy consumers. According to BP statistical review [?], transport is responsible for the consumption of around one fifth of the global energy production. Since virtually all of it (95%) comes from petroleum, it is no wonder that half of the oil production goes straight to transport.

In cities, transport is an essential part of people's lives. People need to move around, be it for work or for pleasure, and goods must be distributed. Moreover, transport shapes cities: the infrastructure needed for vehicles to run—roads, railways, tunnels, etc.— must be taken into account by city planners. However, cities are points of large concentration of people, and any inconvenience caused by transport will affect a lot of people.

## 2.1 Journeys and vehicles

In order to be able to evaluate the impact of transport, it is necessary to know how much journeys the citizens do during the day. In the particular case of Barcelona, there is very useful data about the journeys the citizens of Barcelona make, as well as those journeys with origin or destination in Barcelona.

### 2.1.1 Main destinations

In [TABLE], the main destinations of the journeys of the residents of Barcelona with origin in Barcelona are presented [?]

The round-trip distance between Barcelona and those towns has been estimated as follows:

1. The road distance ($d_R^i$) between Barcelona and the town $i$ has been calculated using Google Maps, taking the first occurrence as the most quick.

2. The straight distance ($d_S^i$) between Barcelona and the town $i$ has been measured using Google Maps as well.

Table 2.1: Main destinations

| Municipality | Journeys | Ratio [%] |
|---|---|---|
| Hospitalet de Llobregat(L') | 42359 | 14.9 |
| Cerdanyola del Vallès | 16991 | 5.99 |
| Prat de Llobregat (El) | 15903 | 5.60 |
| Badalona | 15536 | 5.48 |
| Sant Cugat del Vallès | 12570 | 4.43 |
| Esplugues de Llobregat | 10424 | 3.67 |
| Cornellà de Llobregat | 10331 | 3.64 |
| Sabadell | 6920 | 2.44 |
| Terrassa | 6859 | 2.42 |
| Sant Adrià de Besòs | 6251 | 2.20 |
| Santa Coloma de Gramenet | 5839 | 2.06 |
| Other RMB[1] towns | 99679 | 35.13 |
| Out of RMB | 34097 | 12.02 |
| TOTAL | 283759 | 100 |

[1]Regió Metropolitana de Barcelona

3. The ratio between road distance and straight distance has been calculated and averaged over all towns ($\bar{\rho}$).

4. The distance from the center of each town—including Barcelona—is estimated from their area ($A_i$) (taken from their respective wikipedia [?] pages) as if the towns were circular. That is,

$$r_i = \sqrt{A/\pi} \tag{2.1}$$

5. The corrected radius is calculated multiplying the radius by the mean road-straight ratio:

$$r'_i = r_i \, \bar{\rho} \tag{2.2}$$

6. Finally, the total round-trip distance ($d^i_{RT}$) is calculated with the [EQUATION]

$$d^i_{RT} = 2\,(d^i_R + r'_i + r'_{BCN}) \tag{2.3}$$

[TABLE] presents the estimated round-trip distance of all the towns—except other RMB towns and out of RMB towns—, as well as the ratio of journeys that are below that distance.

Those distances will be used to choose the target range of the vehicle.

Table 2.2: Estimated round-trip distances

| Municipality | Round-trip distance [km] | Ratio of shorter journeys [%] |
|---|---|---|
| Esplugues de Llobregat | 38 | 3.7 |
| Sant Adria de Besos | 38 | 5.9 |
| Hospitalet de Llobregat (L') | 39 | 20.8 |
| Santa Coloma de Gramenet | 43 | 22.9 |
| Badalona | 47 | 28.3 |
| Cornell de Llobregat | 50 | 32.0 |
| Prat de Llobregat (El) | 52 | 37.6 |
| Sant Cugat del Valls | 65 | 42.0 |
| Cerdanyola del Valles | 70 | 48.0 |
| Sabadell | 86 | 50.4 |
| Terrassa | 101 | 52.9 |

### 2.1.2 Hourly distribution of journeys

The information about how many cars are driving in the city at a given time is very valuable, also. It will allow us to evaluate the environmental impact, as well as the social impact.

The number of circulating cars is estimated from the hourly distribution of journeys of the residents of Barcelona [FIGURE] [**?**], assuming that the hourly distribution of all the journeys to and/or from Barcelona is the same.

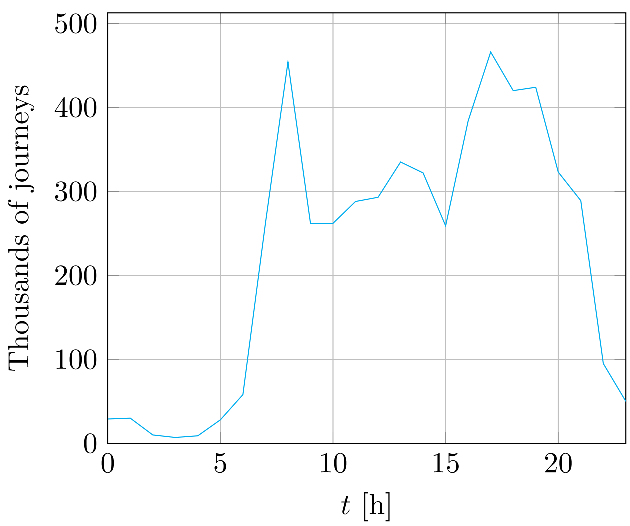


Figure 2.1: Hourly distribution of the journeys of the residents of Barcelona

Let $j(t)$ be the number of journeys of the residents of Barcelona at time $t$. The, the estimated number of cars $N_c(t)$ circulating in Barcelona at time $t$ is:

$$N_c(t) = j(t)\frac{N_{tot}}{N_{res}}\, s_p\, s_c\, f_o^{-1} \tag{2.4}$$

The parameters used are those of [TABLE] and are taken from [**?**].

Table 2.3: Journeys and factors

| Parameter | Symbol | Units | Value |
|---|---|---|---|
| Total no. of journeys[1] | $N_{tot}$ | thousands | 6558 |
| No. of journeys residents | $N_{res}$ | thousands | 5359 |
| Private transport share | $s_p$ | % | 23.1 |
| Car share (of private) | $s_c$ | % | 69.8 |
| Occupation factor | $f_o$ | passenger/veh | 1.2 |

[1]From and/or to Barcelona

The estimated number of cars circulating in Barcelona can be seen in [TABLE]. The values of occupation factors other than the actual will be used in the environmental impact section to assess the impact under different scenarios.

Table 2.4: Thousands of cars circulating in Barcelona

| $f_o$ | Min | Mean | Max |
|---|---|---|---|
| 1.2 (actual) | 1.2 | 36.7 | 76.6 |
| 1.5 | 0.9 | 29.4 | 61.3 |
| 2 | 0.7 | 22.0 | 45.9 |

Further, an estimation of the utilisation factor $f_u$ can be calculated as the quotient of the number of circulating cars by the number of cars owned by the residents of Barcelona. Knowing that the number of cars owned by the residents of Barcelona is 564700 [**?**], the maximum utilisation factor is $f_u^{max} = 13.6\,\%$.

## 2.2 Social and environmental issues

There are numerous social and environmental problems arising from road traffic in cities, such as space taken by roads and cars, car crashes, air pollution, etc. In the next lines, the most critical of them, in the author's judgement, are analysed.

### 2.2.1 Space

The space in a city is divided, in broad terms, in built areas and streets. Streets comprise both vehicle-intended areas and pedestrian-intended areas. Finally, vehicle-intended areas can be divided into parking areas and drivable areas.

The occupation of public space by vehicles is undesirable. It subtracts space for its use by citizens and it discourages its use because of noise, pollution and the intrinsic

Table 2.5: Division of space in Barcelona

| Parameters | Units | Value |
|---|---|---|
| Vehicle-intended area | $km^2$ | 11.40 |
| Pedestrian-intended area | $km^2$ | 16.18 |
| Total area | $km^2$ | 102.16 |
| Total street length | km | 1367.97 |
| In-street parking spots | - | 141061 |

danger of nearby road traffic. For those reasons, the trend in the last years has been to decrease the area intended for vehicles in favour of pedestrians. This can be accomplished by reducing the total length of roads—that is, reducing the city areas one can reach by private vehicle—and reducing the mean width. However, the transit capacity of a road largely depends on its width—iėṅumber of lanes—, so reducing street lanes without taking action to reduce traffic might as well collapse the city transport system. As shown in table [TABLE], the ratio of pedestrian-to-vehicle space is $r_s = 1.42$.

The minimum space that a single vehicle needs depends on the width needed to circulate —which is function of the speed—, the vehicle longitude and a safety distance—which is function of the speed, as well. The equation [EQUATION] shows that relation.

$$a_v = w\,(l_v + d_r + d_b)$$

Table 2.6: Necessary width

| Speed [km/h] | $w$ [m] |
|---|---|
| 10 | 2.5 |
| 40 | 3.0 |
| 100 | 3.5 |

The data shown in table [TABLE] can be fitted into a quadratic equation (EQUATION), where $w$ is the necessary width in metres, and $v$ is the vehicle's speed in kilometres per hour. With the average speed of Barcelona ($\bar{v} = 21\,\text{km/h}$) [REF, DB_2014.pdf], the mean necessary width is $\bar{w} = 2.7\,\text{m}$.

$$w(v) = 9.26 \cdot 10^{-5} v^2 + 0.0213 v + 2.3$$

The safety distance between vehicles depends on the reaction time of the driver and the minimum braking distance. The reaction time varies from person to person, but a value of $t_r = 1.5\,\text{s}$ can be used as a representative of the mean driver. The distance the vehicle drives between the time a braking event—for instance, a pedestrian crossing the road unexpectedly—and the time the driver pushes the braking pedal is simply the product of the vehicle's speed and the reaction time (EQUATION). With the mean speed used before, we have a mean reaction distance of $\bar{d}_r = 8.75\,\text{s}$.

$$d_r = v\, t_r$$

The braking distance can be calculated with the work done by the braking force and the loss of kinetic energy of the vehicle. The maximum force exerted by the road surface to the wheels is limited by the friction coefficient of that contact. Wheels dynamics are tricky, and there are no single static and dynamic friction coefficients. Instead, the friction coefficient value depends on the slip of the wheel. The peak value typically lies between 0.9 and 1.1 for dry asphalt, so a value of 1.0 seems a good approximation.

$$W_b = F_b\, d_b = m\, g\, \mu\, d_b$$

A vehicle with mass $m$ driving at speed $v$ has a kinetic energy (EQUATION) and the braking work must equal that energy in order to completely stop the vehicle.

$$E_k = \frac{1}{2}\, m\, v^2$$

Combining equations (EQUATION) into (EQUATION), and using the average speed, the mean braking distance is $\bar{d}_b = 1.73\,\mathrm{m}$.

$$d_b = \frac{v^2}{2\, \mu\, g}$$

Using an average vehicle length of $l = 4\,\mathrm{m}$, the average area a driving vehicle needs in Barcelona is $\bar{a}_v = 39.1\,\mathrm{m}^2/\mathrm{veh}$.

Knowing this, the total drivable area $A_D$ and the number of driving vehicles, we can calculate a *road occupation index*, or $I_{RO}$, which we can use to calculate the needed vehicle-intended area if we change some parameters, such as the number of vehicles, the average speed, etc.

$$I_{RO} = \frac{a_v\, N_v}{A_D}$$

Table 2.7: default

| | min | avg | max |
|---|---|---|---|
| Number of vehicles | | | |
| Road occupation index | | | |

### 2.2.2 Noise

Cities are noisy and mostly due to road traffic. Even though the roaring sound of cars is caused by both rolling noise and engine noise, at low speeds the engine noise dominates. It is so, that there is a debate on wether electric vehicles should emit an artificially added sound, and what sound should it be; electric vehicles are so quiet that pedestrian do not notice them.

Not only a noisy environment is annoying, but it can be unhealthy. Hearing impairment, hypertension, ischemic heart disease, sleep disturbance,... the litany of diseases linked to noise exposure is long, so reducing noise should be a priority.

Sound is the vibrations that travel through the air as pressure waves. Sound pressure is the local differential pressure compared to the normal ambient pressure.

$$L_p = 20\log(\frac{P}{P_0}) \tag{2.5}$$

An experimental expression of road traffic noise is given in [EQUATION] [**?**]. The sound pressure level depends on the speed of the vehicles ($v$), the traffic intensity ($q$), and the distance from the centre of the road to the listener ($d$).

$$L_p = 26.7\,\log v + 10\,\log q - 10\,\log d + 5.5 \tag{2.6}$$

From [EQUATION], we deduce that if, for instance, half of the vehicles of a road were suddenly noiseless, the sound pressure level would be reduced to:

$$\frac{L_{p2}}{L_{p1}} = 1 + \log(\frac{q_2}{q_1}) \rightarrow L_{p2} = 0.7\,L_{p1} \tag{2.7}$$

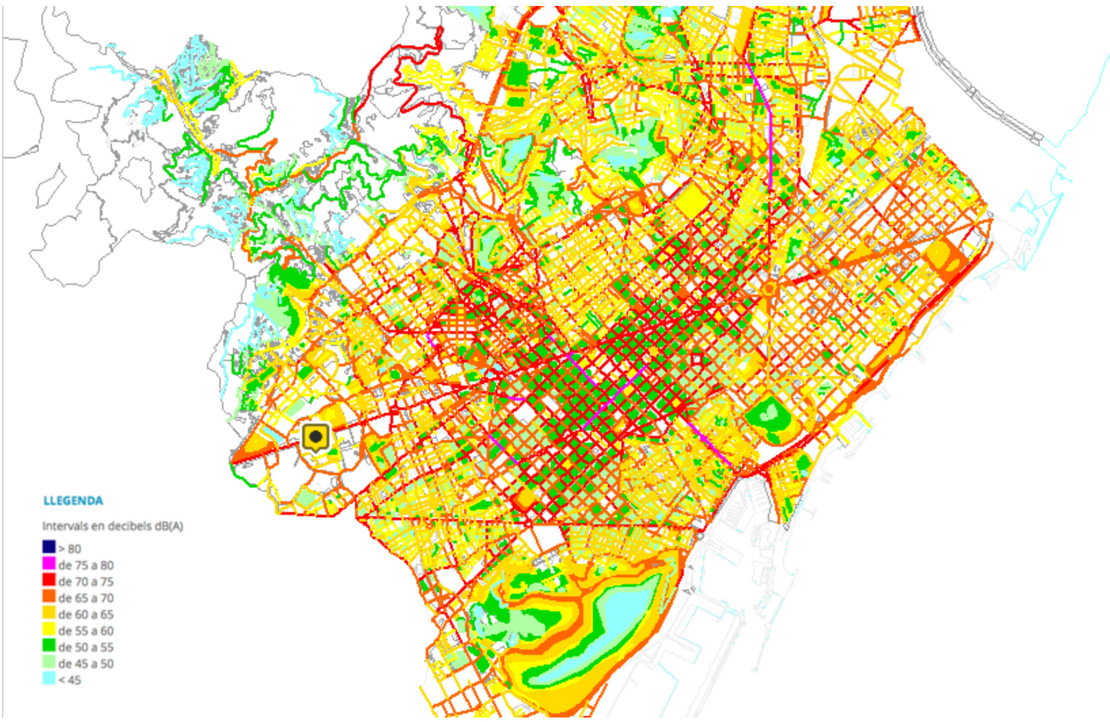


Figure 2.2: Sonic map of Barcelona

### 2.2.3 Air quality

Air is essential to us, and a low quality air—as it is in most big cities—has proven detrimental to the citizens' health. Since most of industries moved away form city centres, the main cause of air pollution in cities is road traffic.

Carbon dioxide ($CO_2$) is a pollutant, but is not directly harmful to humans, or at least at today's levels. Apart from it, there are many pollutants emitted by fossil-fueled vehicles which concentration in some cities is alarming. Some of those pollutants are:

- Carbon monoxide (CO)
- Unburnt or evaporated hydrocarbons (HC)
- Nitrogen oxydes (NOx)
- Lead (Pb)
- Sulphur dioxide ($SO_2$)
- Tropospheric ozone ($O_3$)

In Catalonia, the index used to measure the quality of air is the *Índex Català de la Qualitat de l'aire* (ICQA). This index can have values from -100 to 100. It is a qualitative measure of the air quality, based on concentrations of tropospheric ozone, particulate matter (PM10), carbon monoxide, sulphur dioxide, and nitrogen dioxide. The values for each pollutant are computed according to their risk posed on human health. The overall value is the minimum of each pollutant. An ICQA greater than 50 means a good quality air, between 0 and 50 indicates regular quality air, and a value below zero implies bad quality air. The mean values of the ICQA of Barcelona of the last years are listed in [TABLE][SOURCE idescat].

Table 2.8: Values of the ICQA of Barcelona

| Year | 2010 | 2011 | 2012 | 2013 | 2014 | 2015 |
|---|---|---|---|---|---|---|
| Minimum value | 0 | -8 | -7 | -8 | -56 | -52 |
| Maximum value | 97 | 91 | 93 | 91 | 97 | 92 |
| Average value | 52 | 57 | 58 | 55 | 56 | 51 |

## 2.3 Mitigation measures

Now that we have seen, not all, but some of the problems caused by road traffic in cities, here are some possible actions to reduce them.

**Increase powertrain efficiency**: This is the main topic of this thesis, so it does not need further comment.

**Self-driving vehicles**: Self-driving—or autonomous—vehicles will reduce the accident rate, allow more traffic intensity with less speed, and pave the way to get rid of the cultural *need* of owing a vehicle.

**Coordinated vehicles**: Related to autonomous vehicles, a coordination system with real-time traffic information would reduce, amongst other things, the trip time and the overall energy consumption—by reducing the number of stops in a journey.

**Car-sharing and car-pooling schemes**: Sharing vehicles would reduce significantly the number of vehicles present in the city. Hence, the overall energy consumption will be lower—we would not need to manufacture so many vehicles—and a lot of space would be recovered. In fact, there are many initiatives in this line all over the world, both private and public funded.

**Occupational mobility**: Most of journeys take place because people usually work too far away from home. Promoting work-from-home schemes could drastically reduce the number of journeys. Also, reducing the number of weekly work days would have a similar effect, even though it could also increase the number of leisure-related journeys.

**Distributed leisure centres**: People living in degraded or residential neighbourhoods use the car much more often than people living in city centres. Therefore, actively promoting the restoration of degraded zones and the distribution of journey attractors would discourage motored transport in favour of walking.

# Chapter 3

# The vehicle

This chapter presents the preamble of the search for the most sustainable propulsion system. First, longitudinal vehicle dynamics are analysed so that we can model the basic behaviour of the vehicles under different circumstances. Also, the vehicles' components are studied.

## 3.1 Vehicle dynamics

There are forces that act on a vehicle which oppose its movement. Those forces are called resistive forces ($F_r$). Resistive forces are the aerodynamic drag, the rolling resistance, and the grading resistance. On the other hand, the wheels exert a force– the tractive force, $F_t$—on the road. If the tractive force overcomes the resistive force, the vehicle accelerates; if it is lower, the vehicle decelerates; and if it equals the resistive force, the vehicle is kept at a constant speed.

$$F_t - F_r = M \cdot a$$

The tractive force is transmitted from the powertrain to the wheels—or from the brakes when braking. So, in order to know the needed tractive force at any given time, a model of the resistive forces is needed. In the following points, the resistive forces are analysed and a vehicle dynamics equation is provided. This equation will be used later in the simulations.

### 3.1.1 Aerodynamic drag

Aerodynamic drag—sometimes called air resistance—is a force exerted by a flowing gas on a body. The direction of this force is the direction of the fluid freestream flow, that is, the direction of the flow seen from the body. It is caused by, mainly, pressure distributions over the body and viscous forces due to skin friction.

An exact calculation of the aerodynamic drag is virtually impossible due to the complexity of a vehicle's geometry. However, given the expression [EQUATION] the drag coefficient $C_d$ can be calculated from wind tunnel measures.

$$F_{ae} = \frac{1}{2}\rho A_f C_d v^2$$

In the expression above, $F_{ae}$ is the aerodynamic drag force, $\rho$ is the air's density, which has a value of $\rho = 1.225$ kg/m$^3$ at sea level, $A_f$ is the frontal area, $C_d$ is the drag coefficient, and $v$ is the relative velocity of the air. The relative velocity of the air depends on the vehicle speed and the wind speed. Since the wind speed is unknown at the time of designing a vehicle, largely unpredictable at any given time, and mostly random over the lifetime of the vehicle, it is usually neglected, and the vehicle speed alone is used instead.

When designing a vehicle, the only two factors that can be modified are the drag coefficient and the frontal area of the vehicle. The parameters used can be found in [TABLE].

Table 3.1: Aerodynamic parameters

| Parameter | Symbol | Units | Value |
|---|---|---|---|
| Air density | $\rho$ | kg/m3 | 1.225 |
| Frontal area | $A_f$ | m$^2$ | 2.1 |
| Drag coefficient | $C_d$ | – | 0.3 |

### 3.1.2 Rolling resistance

Rolling resistance is a force resisting the motion of a body rolling on a surface. In the context of vehicles, rolling resistance is the force acting on the wheels.

Wheels are not perfectly circular: under their own weight and the weight of the vehicle they deform adopting a flat area in the contact with the road. Thus, when the vehicle advances, the wheel must be reshaped. Due to the viscoelastic characteristics of the rubber of the wheel, the energy needed to deform it is greater than the energy released when it recovers its original shape, i.e. it presents hysteresis. The difference between those energies is transformed into heat and it cannot be recovered.

The rolling resistance force depends on the vertical force on the wheel, $F_z$, and the rolling resistance coefficient, $f_r$:

$$F_{rr} = f_r F_z$$

The vertical force on each wheel varies greatly during a journey. Plus, the vertical load of the vehicle is influenced by the aerodynamic lift: in racing and sports cars, the vertical load increases with speed to provide stability and grip; in passenger cars, the vertical load decreases with speed to alleviate the overall load. However, for the sake of simplicity, we can assume that, on average, the vertical force is evenly distributed over all wheels, and it does not vary with speed. Then, the vertical load of the whole vehicle has the expression of [EQUATION], where $m$ is the vehicle's mass, and $\alpha$ is the slope angle of the road.

$$F_z = mg \sin\alpha$$

The rolling resistance coefficient depends on a lot of factors, so it is not worth trying to elaborate a theoretical model. Instead, we can rely on experimental results. For a typical passenger car, and up to a speed of 150 km/h, the rolling resistance coefficient varies with the speed according to this expression:

$$f_r = 0.0136 + 0.4 \cdot 10^{-7} v^2 \text{ [N] } (v \text{ in km/h})$$

According to this expression, the rolling resistance coefficient is only 6.6% larger at a speed of 150 km/h than it is when stopped. Therefore, the results will not vary greatly if it is assumed to have a constant value. Typical values for a passenger car on asphalt found in the literature are around $f_r = 0.015$. However, [**?**] limits this parameter to $f_r = 0.0105$. Therefore, this is the value used. To sum up, the expression of the rolling resistance force is:

$$F_{rr} = f_r mg \cos\alpha$$

### 3.1.3 Grading resistance

When the vehicle goes in a non-horizontal road, the component of weight parallel to the surface is directed downwards and opposes the vehicle motion—when uphill—or helps it—when downhill. The expression of this force is that of [EQUATION], where $\alpha$ is the slope angle.

$$F_g = mg \sin\alpha$$

It is usual to give the slope grades in percentages. In this case, the angle can be calculated as follows:

$$\alpha = \arctan \frac{\text{grade[\%]}}{100}$$

Road planners have that in mind when designing the alignment of the road, so we do not find extreme uphill or downhill angles. In general, the maximum values depend on the type of road, the speed of the road, where it is, etc. Maximum values of slope in Spain are given in [TABLE] [**?**].

| Road | Grade |
|---|---|
| Motorway | 4% |
| Expressway | 7% |
| Ordinary road | 18% |
| Mountain pass road | 25% |

Table 3.2: Typical maximum slope for different roads in Spain

### 3.1.4 Inertial forces

A vehicle rarely goes at a constant speed, so it needs to be able to accelerate. Here is when the famous equation of the Newton's second law of motion comes in:

$$F = m\frac{dv}{dt}$$

That is, of course, supposing the vehicle does not lose mass—which it does. Nevertheless, the mass loss is negligible, so we can confidently use this equation.

Even so, the kinetic energy of the vehicle is not only the kinetic energy due to its mass and speed. In any vehicle, there are rotating parts that have kinetic energy as well. Those parts are, mainly, the engine, motor, clutch, gearbox, axles, wheels, and brake disks. Each of those $N$ elements, $i$, has a moment of inertia $J_i$, and rotates at a given speed $\omega_i$, which is related to the vehicle speed $v$ with a certain radius $r_i$. Then, the total amount of kinetic energy is given by the expression:

$$E_c = \frac{1}{2}mv^2 + \frac{1}{2}\sum_i^N J_i\omega_i^2 = \frac{1}{2}mv^2 + \frac{1}{2}\sum_i^N J_i r_i^{-2} v^2 = \\ = \frac{1}{2}(m + \sum_i^N J_i r_i^{-2})v^2$$

So, we could say that the vehicle has the same kinetic energy that a body of mass $M$ at the same speed, where

$$M = m + \sum_i^N J_i r_i^{-2} = (1+\epsilon)m$$

Since it would be a tedious work to calculate the moment of inertia and the radius of each rotating mass, an equivalent mass factor $\epsilon$ is more convenient. Typical values of the mass factor can be seen in [TABLE] [**?**].

Table 3.3: Typical values of the mass factor

| Vehicle | Short gear | Long gear |
|---|---|---|
| Small vehicle | 0.25 | 0.05 |
| Large vehicle | 0.40 | 0.07 |

In general, electric vehicles have less rotating masses than internal combustion engine vehicles, so the equivalent mass factor should be lower. The values used are shown in [TABLE].

Table 3.4: Values of equivalent mass factor used

| Vehicle | $\epsilon$ |
|---|---|
| Vehicles with ICE | 0.25 |
| Purely electric propulsion vehicles | 0.1 |

### 3.1.5 Longitudinal vehicle dynamics

We have seen the forces that oppose to the movement of the vehicle. The sum of those forces is the resistive force [EQUATION]. To overcome the resistive force, the powertrain must provide power to the wheels.

$$F_r = F_{ae} + F_{rr} + F_g$$

Therefore, the tractive force minus the resistive force is the net force, which makes the vehicle accelerate—if positive [EQUATION].

$$F_t - F_r = M\frac{dv}{dt}$$

Sometimes it is more convenient to use powers instead of forces. In terms of power, the above equation can be written as:

$$P_t - P_r = \dot{E}_c \rightarrow F_t v - F_r v = Mv\frac{dv}{dt}$$

## 3.2 Vehicle components

A typical vehicle is made of thousands of parts. Based on [Buhrnam2012], we have grouped those parts in three main categories: body, energy storage systems and powertrain.

**Energy storage system**: Fuel storage system, batteries, ultracapacitors, flywheels.

**Powertrain**: Engine, motor, transmission, fuel cell stack.

**Body**: The rest of the vehicle.

In this document [**?**], the mass of each component, as well as its material composition, is specified for different types of vehicles. Unless otherwise specified, the data used in the models is from the document mentioned.

### 3.2.1 Vehicle assembly

Besides the energy and emissions of the extraction of materials—which we have seen in [SECTION]—and the energy and emissions of the components manufacturing, the vehicle needs to be assembled and that also consumes energy and emits GHG.

| Parameter | Value |
|---|---|
| Fossil energy [MJ/kg] | 4.66 |
| Total energy [MJ/kg] | 8.88 |
| GHG emissions [kg $CO_2$e/kg] | 0.58 |

Table 3.5: Energy requirements and emissions for the vehicle assembly

### 3.2.2 Body

In this context, the body is the whole vehicle without the powertrain and the energy storage systems. It includes everything that is necessary to operate it.

The design of this part is not the object of this thesis, so base case numbers will be used in order to design the propulsion system around the body. To do so, a set of mini cars—A-segment vehicles—has been analysed to find a body base weight. Also, an estimation of the powertrain specific power has been made for internal combustion engine vehicles (ICEV). This analysis can be found in Annex $\kappa$ [ANNEX]

The body mass is 500 kg. The total vehicle mass will be the body mass, plus the powertrain and energy storage systems masses, and the driver.

The material composition of the vehicle without powertrain and energy storage systems is presented in [TABLE]. Then, the weighed average of the materials and their energy requirements and greenhouse gases emissions gives us the specific energy requirements of the body, as shown in [TABLE]

Table 3.6: Material composition of the body

| Material | Mass [%] |
|---|---|
| Steel | 73.2 |
| Plastic | 11.5 |
| Glass | 4.3 |
| Rubber | 3.3 |
| Iron | 2.4 |
| Copper | 1.7 |
| Paint | 1.3 |
| Fabrics | 1.2 |
| Aluminium (wrought) | 0.8 |
| Friction material | 0.2 |
| Magnesium | 0.026 |
| Zinc | 0.011 |
| Others | 0.015 |

Table 3.7: Energy requirements and emissions of the body

| Component | Energy [MJ/kg] | GHG emissions [kg $CO_2$e/kg] |
|---|---|---|
| Body | 60.97 | 4.3 |

### 3.2.3 Electric motors

Electric motors are electromechanical energy converters, that is, they are devices that convert electrical energy into mechanical energy. In the scope of vehicles, electric motors transform the electricity stored in the vehicle in some way into kinetic rotational energy. This energy is transferred to the wheels, which make the vehicle move.

Table 3.8: Electric motor characteristics

| Parameter | Symbol | Value |
|---|---|---|
| Motor performance | $\eta_m$ | 90% |
| Specific power [?] | $p_m$ | 1.44 kW/kg |
| Power-to-torque ratio | $r_P^\Gamma$ | 0.005 N m/W |
| Maximum speed | $n_{max}$ | 6000 min$^{-1}$ |
| Regenerative braking ratio | $n_{RB}$ | $12^{-1}$ |
| Converter specific power | $p_c$ | 14.1 kW/kg |

There are several types of electric motors, but our interest is not to choose one yet. Instead, we will use a general model of an electric motor, consisting in an energy converter with a given efficiency. The table [TABLE] presents the values of the generic model.

The mass of the chosen motor will be the product of its maximum power by the motor specific power. The motor is sized by its power, so a power-to-torque ratio is used to calculate the maximum torque. The regenerative braking ratio is the ratio of the maximum speed at which regenerative braking can function at full. At low speeds, the generator cannot efficiently produce negative torque, so that parameter is used to model this effect. Finally, the converter of the motor is also included. Its mass is the product of the motor max power by the converter specific power. The losses of the converter are not modelled.

The material composition of the motor is shown in [TABLE]. That leads to the energy and emissions associated to its manufacture of [TABLE].

Table 3.9: Material requirements of an electric motor

| Material | Mass[%] |
|---|---|
| Steel | 36.1 |
| Aluminium (cast) | 36.1 |
| Copper | 27.3 |

Table 3.10: Energy requirements and emissions of an electric motor

| Parameter | Value |
|---|---|
| Fossil energy [MJ/kg] | 60.66 |
| Total energy [MJ/kg] | 75.73 |
| GHG emissions [kg $CO_2$e/kg] | 5.85 |

### 3.2.4 Internal combustion engines

Internal combustion engines (ICE) are heat engines where the combustion of a fuel occurs in the working fluid flow circuit. There are several types of ICE, but virtually all cars use four-stroke engines, either spark-ignited (Otto cycle) or compression-ignited (Diesel cycle). In an ICE, the chemical energy stored in the bonds of the fuel's molecules is converted into kinetic rotational energy. Since we have only studied petrol, and not diesel fuel, henceforth ICE refers to four-stroke spark-ignited engine.

The overall efficiency of an ICE is the ratio of brake power to fuel power:

$$\eta_e = \frac{\Gamma_b \cdot \omega_m}{\dot{m}_f \cdot H_f} \tag{3.1}$$

Power losses are due to, mainly, four factors: thermal, volumetric, mechanical, and parasitic losses. Thermal losses account for the heat released by the combustion of the fuel that is not converted into work. It is known that the maximum thermal efficiency of a heat engine is the Carnot efficiency. However, the maximum thermal efficiency of an ICE is even less, and it is given by [EQUATION].

$$\eta_{th} = 1 - \frac{1}{r^{\gamma-1}} \tag{3.2}$$

where $r$ is the compression ratio and $\gamma$ is the specific heat ratio of the gas in the combustion chamber.

Volumetric—or pumping—losses are a consequence of pressure-gradient-induced forces acting on the piston that oppose normal piston movement. In the intake stroke, the piston draws air from the intake inlet. Volumetric efficiency is the ratio of the volume of air drawn into the piston at atmospheric pressure to the volume of the cylinder. Equally, volumetric efficiency also affects the exhaust stroke, leaving some of the exhaust gases inside the cylinder.

Mechanical losses are due to the friction between moving parts of the engine. Mainly, they are caused by the friction at the ring-cylinder interface and at the crankshaft bearing assemblies.

Lastly, parasitic losses account for the power needed to run the ancilliaries: oil and coolant pumps, power steering, alternator, etc.

$$\eta_e = 1 - \frac{P_{l,th} - P_{l,v} - P_{l,m} - P_{anc}}{\dot{m}_f \cdot H_f}$$

The efficiency of electric motors varies with speed and torque, but overall the efficiency is high. Internal combustion engines, though, have very poor efficiencies. Moreover, the object of hybridisation of ICEV, besides regenerative braking, is to ensure the engine works at a high efficiency point. For this reason, the engine model used is more complex, and consists of an energy converter with variable efficiency—which is interpolated from an efficiency map [FIGURE][SOURCE].

The engine is sized from its maximum power. First, the power curve of the engine is calculated from a generic engine torque expression [EQUATION][1] by multiplying the

[1]This curve is a parametric curve that happens to resemble typical engine torque curves. The parameters of the curve have been chosen qualitatively comparing the resulting curve with an actual torque curve.

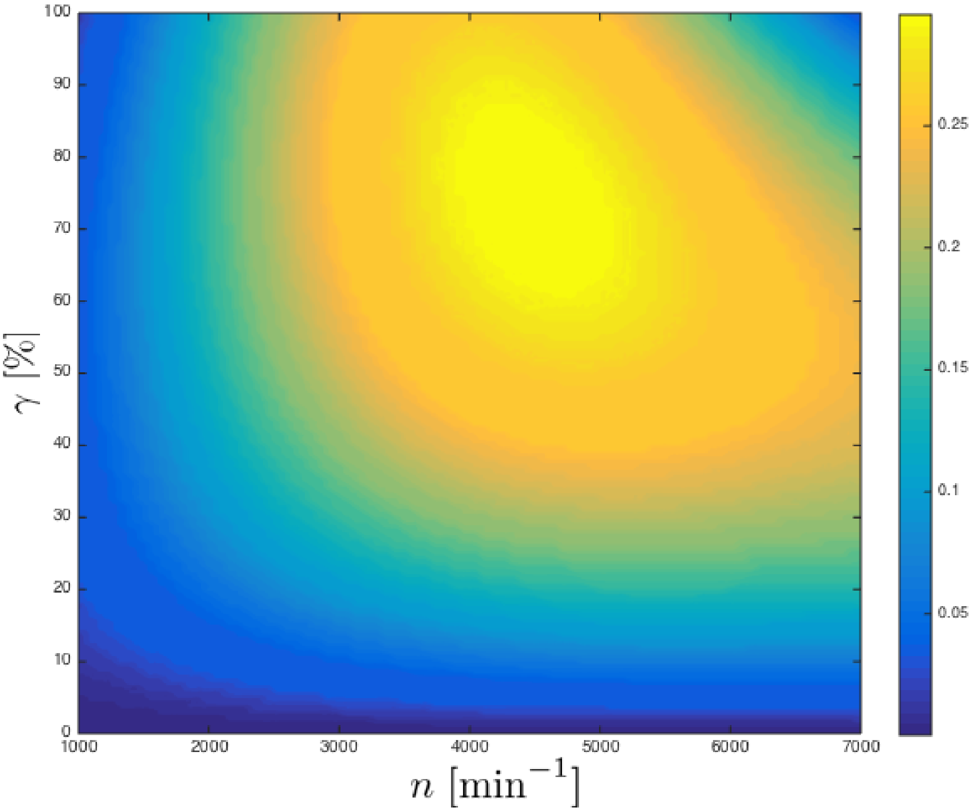


Figure 3.1: Efficiency map of the ICE

curve by the engine speed. Then, the power curve is scaled up for the maximum power of the curve to match the maximum power desired. Finally, the maximum torque speed is computed, then the maximum torque, and the torque curve is scaled up.

$$\Gamma_n = -e^{a\,(\omega_n - b)} + a\,(\omega_n - b) + c \tag{3.3}$$

The engine efficiency map is rectangular, but the operative zones of the engine are not. Therefore, it is necessary to position the torque curve on the efficiency map. This has been made by overlapping the sweet spots of the two data. On the efficiency map, the sweet spot is simply the point of maximum efficiency. On the torque-speed map, the sweet spots occurs at the speed of maximum torque and at the torque at around 80% of the maximum. The y-axis of [FIGURE], $\gamma$ is the ratio between torque and absolute max torque.

Table 3.11: Engine torque curve parameters

| Parameter | Value |
|---|---|
| $a$ | 1.4 |
| $b$ | 0.5733 |
| $c$ | 2 |

Table 3.12: Engine parameters

| Parameter | Symbol | Units | Value |
|---|---|---|---|
| Minimum speed | $n_{min}$ | $\mathrm{min}^{-1}$ | 1000 |
| Maximum speed | $n_{max}$ | $\mathrm{min}^{-1}$ | 7000 |
| Specific power | $p_e$ | kW/kg | |

### 3.2.5 Transmission

The transmission is an essential part of a vehicle, as it adapts the torque and speed form the motor to the wheels. A defective designed transmission would translate into poor drivability and low performance.

An internal combustion engine requires a multi-speed transmission, because the torque it produces is highly dependent on its speed. Furthermore, the engine must be kept above its minimum speed, so a coupling device—a clutch or a torque converter—must be used to allow the vehicle operate from still.

In regard of transmission requirements, electric motors are much less demanding than ICE. The torque curve of a motor is much flatter than that of an ICE, and it can, in most cases, produce torque at zero speed. Therefore, a single ratio transmission is usually enough.

Consequently, a continuously variable transmission (CVT) and a torque converter will be used with ICE, and a single ratio transmission with electric motors. The torque converter model is an energy converter based on [**?**]. The torque output multiplication, or torque ratio (TR), depends on de speed ratio—the difference between the two shafts—as we can see in [FIGURE]. The torque boost comes at the expense of efficiency, which is the product of both ratios [EQUATION]

$$\omega_o = \mathrm{SR}\,\omega_i \tag{3.4}$$

$$\Gamma_o = \mathrm{TR}\,\Gamma_i \tag{3.5}$$

$$\eta = \frac{P_o}{P_i} = \frac{\Gamma_o\,\omega_o}{\Gamma_i\,\omega_i} = \mathrm{SR}\cdot\mathrm{TR} \tag{3.6}$$

### 3.2.6 Fuel cells

Fuel cells are galvanic cells in which the chemical energy of a fuel is converted directly into electrical energy [Ehsani]. Fuel cells do not store energy; rather, they are energy

| Material | Mass[%] |
|---|---|
| Steel | 50.4 |
| Aluminium (cast) | 14.7 |
| Plastic | 10.0 |
| Iron (cast) | 9.8 |
| Aluminium (wrought) | 6.8 |
| Copper | 3.1 |
| Stainless steel | 2.9 |
| Rubber | 2.4 |
| Platinum | 0.002 |

Table 3.13: Lightweight ICE powertrain material requirements.

| Parameter | Value |
|---|---|
| Fossil energy [MJ/kg] | 63.97 |
| Total energy [MJ/kg] | 78.80 |
| GHG emissions [kg $CO_2$e/kg] | 5.78 |

Table 3.14: Lightweight ICE powertrain energy requirements and emissions

converters. The energy comes from a fuel, so it has to be stored. The main fuel used in fuel cells is hydrogen, which, when used, produces only water [EQUATION]

$$2\,H_2 + O_2 \longrightarrow 2\,H_2O$$

There are six major types of fuel cells:

- Proton exchange membrane fuel cells (PEMFCs, or simply PEM)
- Alkaline fuel cells (AFCs)
- Phosphoric acid fuel cells (PAFCs)
- Molten carbonate fuel cells (MCFCs)
- Solid oxide fuel cells (SOFCs)
- Direct methanol fuel cells (DMFCs)

Of those, PEMFCs are the most widely used in vehicular applications. Fuel cells are seen as green technology, and indeed hydrogen fueled FC only produce water vapor. If the hydrogen is obtained with renewable resources, they are definitely clean. However, PEMFCs present some drawbacks. First, the electrolyte membrane needs a catalyst and, due to the conditions at which the fuel cells needs to run, nobel metals—such as platinum—are the best candidates. Second, water management is a critical issue. The humidity conditions for the cell to work properly are very narrow, and has to be

Table 3.15: CVT and torque converter characteristics

| | |
|---|---|
| CVT ratio range | 5 |
| CVT efficiency | % |

Table 3.16: default

| FC type | Operating temperature | Power | Efficiency[1] |
|---|---|---|---|
| AFC | 90–100 °C | 10–100 kW | 60–70% (E) |
| PAFC | 150–200 °C | 50 kW–1 MW | 80–85% (CHP) 36–42% (E) |
| PEM[2] | 50–100 °C | <250 kW | 50–60% (E) |
| MCFC | 600–700 °C | <1 MW | 85% (CHP), 60% (E) |
| SOFC | 650–1000 °C | 5 kW–3 MW | 85% (CHP), 60% (E) |

[1]CHP: combined heat and power, E: electric

[2]DMFC are a subset of PEM, with powers up to 100 W

controlled properly. Finally, fuel cells can be *poisoned* with other gases that have more affinity with the catalyst, such as carbon monoxide and sulfur products.

The model of the fuel cell used here is a very simplistic approximation consisting of an efficiency curve depending on the power demand. [FIGURE] shows the efficiency map extracted from [**?**]. The fuel cell is sized by its maximum power, and the efficiency map is scaled accordingly.

Fuel cells (PEM):

- Fuel cell stack power density[1]: 1.75 kW/kg

### Materials and manufacturing

| Material | Mass [%] |
|---|---|
| CFRP | 62.8 |
| Aluminium (wrought) | 23.0 |
| PFSA | 5.4 |
| Carbon paper | 5.0 |
| Steel | 1.5 |
| PTFE | 1.4 |
| Carbon/PFSA suspension | 0.6 |
| Platinum | 0.1 |

Table 3.17: Fuel cell stack material composition

[1]Honda FCX Clarity: 1.5 kW/kg [source]; Honda Mirai: 2 kW/kg [source]

| Parameter | Value |
|---|---|
| Fossil energy [MJ/kg] | 384.21 |
| Total energy [MJ/kg] | 646.15 |
| GHG emissions [kg $CO_2$e/kg] | 48.5 |

Table 3.18: Energy requirements and emissions of the fuel cell stack

### 3.2.7 Batteries

Batteries are electrochemical devices consisting of a collection of cells that convert chemical energy into electric energy and vice versa.

Each cell is composed of mainly three elements: the positive and negative electrodes, and the electrolyte where the electrodes are immersed.

The specific energy—i.e. the energy capacity per unit battery weight—is highly dependent on the cell reactants. The theoretical specific energy is:

$$E_{s,th} = \frac{nFV_r}{3.6 \sum M_i} \text{ [Wh/kg]}$$

where $n$ is the number of electrons transferred in the reaction, $F$ is the Faraday constant, $V_r$ is the reversible voltage of the cell, and $\sum M_i$ is the sum of the species involved in the reaction. The actual specific energy, however, is lower since the reactants are only a fraction of the battery weight.

There are plenty of battery technologies; some of them are well-established and others are still in development. Here, we will compare four battery types:

- Lead–acid
- Nickel–Cadmium
- Nickel–metal hydride
- Lithium–Ion

| Type | Energy efficiency [%] | Specific energy [Wh/kg] | Specific power [W/kg] | Cycle life [at 80% DOPC] | Self-discharge [% per 48h] |
|---|---|---|---|---|---|
| Lead–acid | >80 | 35–50 | 250 | 500–1000 | 0.6 |
| Ni–Cd | 75 | 50–60 | 125 | 800 | 1 |
| Ni–MH | 70 | 70–95 | 200 | 750–1200 | 6 |
| Li–ion | >95 | 80–130 | 300 | >1000 | 0.7 |

Table 3.19: Batteries' parameters.

Comparing the data of the tables [TABLE] and [TABLE], not only we see that lithium batteries are the best in terms of performance, but also they do fairly well in

| Type | Energy [MJ/kg] | GHG emissions [kg$CO_2$e/kg] |
|---|---|---|
| Lead–acid | 30.6 | 4.45 |
| Ni–Cd | 148.9 | 10.75 |
| Ni–MH | 214.0 | 19.88 |
| Li–ion | 161.6 | 16.95 |

Table 3.20: Energy requirements and emissions of the batteries' manufacturing

terms of manufacturing energy requirements per energy stored. For this reasons, only lithium ion batteries are used here.

$$E = E_0 - K \frac{Q}{Q - \int_0^t i(\tau)\,\mathrm{d}\tau} + A\, e^{-B \int_0^t i(\tau)\mathrm{d}\tau} \tag{3.7}$$

The battery model is extracted from [?]. It consists of a variable voltage source—which depends on the charge—and a series resistance. [EQUATION] The parameters for lithium–ion batteries are also extracted from [?] and are listed in [TABLE].

Table 3.21: Li–ion cell model parameters

| Parameter | Symbol | Units | Value |
|---|---|---|---|
| Cell nominal voltage | $V_N$ | V | 3.6 |
| Charge | $Q$ | Ah | 1 |
| Voltage constant | $E_0$ | V | 3.7348 |
| Internal resistance | $R$ | Ω | 0.09 |
| Polarisation voltage | $K$ | V | $8.76\,10^{-3}$ |
| Voltage drop of exponential zone | $A$ | V | 0.468 |
| 3/Charge at the end of exponential zone | $B$ | $(\mathrm{Ah})^{-1}$ | 3.5294 |

The battery is sized according to its energy capacity and voltage, as shown in [EQUATIONS]. To protect battery from being fully discharged, a maximum depth-of-discharge (DoD) is allowed. Also, to prevent overcharging, a maximum state-of-charge is set, so that the battery always has a safe charge. Besides damaging the battery, not respecting this limits can be quite dangerous, as lithium-ion batteries can catch fire, or even explode. State-of-charge and depth-of-discharge are two related values, and are calculated as follows:

$$\mathrm{SoC} = \frac{\int_0^t i(\tau)\mathrm{d}t}{Q} \tag{3.8}$$

$$\mathrm{DoD} = 1 - \mathrm{SoC} \tag{3.9}$$

### 3.2.8 Ultracapacitors

Ultracapacitors—or supercapacitors—are, as it can be guessed by its name, large capacitors, or high-capacitance capacitors. Similarly to other electric components, an

Table 3.22: Battery parameters

| Parameter | Symbol | Units | Value |
|---|---|---|---|
| Specific energy | $e_b$ | Wh/kg | 100 |
| Battery nominal voltage | $U_{bN}$ | V | 400 |
| Battery maximum SoC | $\mathrm{SoC}_{max}$ | | 0.9 |
| Battery maximum DoD | $\mathrm{DoD}_{max}$ | | 0.2 |
| Battery cycle life | $N_C$ | | 1000 |

ultracapacitor is more of a theoretical concept than a particular device. However, when people speak about ultracapacitors, they usually refer to the particular device that behaves like a large capacitor. In the present, ultracapacitors are double-layer capacitors. Ultracapacitors use an electric double layer as insulation, unlike regular capacitors that use plastic or aluminium oxide films. Ultracapacitors present power densities that no battery technology can compete with. However, the limiting factor of energy density due to the maximum voltage that can be achieved [EQUATION], makes them deficient energy storage devices. Combining them with a good energy storage device, can make a very good energy storage system, though.

$$E_c = \frac{1}{2} C\, V^2 \tag{3.10}$$

The model of the ultracapacitor is a capacitor with a series resistance and a parallel resistance that models the leakage current. The equations [EQUATIONS] show the electric relations of an ultracapacitor, where subindices $t$, $C$, and $L$ stand for terminal, capacitor, and leakage, respectively.

$$V_t = V_C - i_t\, R_s \tag{3.11}$$

$$i_C = -C \frac{\mathrm{d}V_C(t)}{\mathrm{d}t} \tag{3.12}$$

$$i_L = \frac{V_C}{R_L} \tag{3.13}$$

$$i_t = i_C + i_L \rightarrow i_t = \frac{V_C}{R_L} - C\frac{\mathrm{d}V_C}{\mathrm{d}t} \tag{3.14}$$

$$\tag{3.15}$$

The parameters used are taken from one particular device, the Maxwell K2 ultracapacitor cell, and are listed in table [TABLE].

### 3.2.9 Flywheels

Flywheels are mechanical devices that store rotational kinetic energy. As we can see from the expression of that energy [EQUATION], there is a parallelism with the expression

Table 3.23: Ultracapacitor cell parameters

| Parameter | Symbol | Units | Value |
|---|---|---|---|
| Capacitance | $C$ | F | 3500 |
| Rated capacitor voltage | $V_{CR}$ | V | 2.85 |
| Series resistance | $R_s$ | m$\Omega$ | 0.22 |
| Leakage resistance[1] | $R_L$ | $\Omega$ | 158.3 |
| Maximum current | $i_{t,max}$ | A | 2000 |
| Mass | $m_{cell}$ | kg | 0.520 |
| Cycle life | $N_c$ | | $10^6$ |

[1] Calculated from a leakage current of $i_L = 18\,\text{mA}$ and the rated voltage

Table 3.24: default

| Parameter | Value |
|---|---|
| Fossil energy [MJ/kg] | – |
| Total energy [MJ/kg] | 98.8 |
| GHG emissions [kg $CO_2$e/kg] | 5.25 |

of the capacitor energy. The correspondence between variables is very straightforward: the moment of inertia $J$ is the capacitance $C$, and the rotational speed $\omega$ is the voltage $V_C$. It is clear then, why flywheels are often referred to as mechanical capacitors.

$$E = \frac{1}{2} J \omega^2$$

A higher energy capacity of flywheels can be achieved by either increasing its moment of inertia or increasing its rotational speed. In stationary applications, where the weight is not crucial, flywheels are usually heavy and slow. However, for its use in vehicles, weight is a key parameter. However, high rotational speeds imply high centrifugal forces which in turn imply high tensile stress. Ultra-high-speed flywheels are designed to rotate at the maximum speed that the material allows before failing.

The specific energy depends on the shape of the wheel and is proportional to the tensile strength to density ratio:

$$e \propto \frac{\sigma}{\rho}$$

Typical materials, such as metals, or plastics, have a rather low tensile strength. The most suitable materials for this application are fiber reinforced polymers, which have a great tensile strength thanks to the fibers, whilst keeping the density low thanks to the polymer. Carbon fiber reinforced polymers are a great candidate for manufacturing ultra-high-speed flywheels.

The model used here is derived from a real flywheel named *flywheel capacitor* manufactured by the association of Magneti Marelli with Flybrid Systems. It is an ultra-high-speed flywheel coupled with an electric motor, which allows for direct electric energy supply. The characteristics of this device are listed in [TABLE] [**?**].

Table 3.25: Flywheel Capacitor characteristics

| Parameter | Symbol | Units | Value |
|---|---|---|---|
| Total mass | $m_{device}$ | kg | 27 |
| Flywheel mass | $m_{fw}$ | kg | 5 |
| Maximum speed | $n_{max}$ | $\min^{-1}$ | 60000 |
| Self-discharge time | $t_{sd}$ | min | 15 |
| Usable energy | $E_u$ | kJ | 530 |
| Electric motor power | $P_e$ | kW | 60 |

**Energy requirements and emissions**

| Parameter | Value |
|---|---|
| Fossil energy [MJ/kg] | 101.71 |
| Total energy [MJ/kg] | 133.80 |
| GHG emissions [kg $CO_2$e/kg] | 9.34 |

Table 3.26: Flywheel energy requirements and emissions. [FLYBRID]

### 3.2.10 Fuel tanks

Fuel tanks are safe containers of flammable fluids, either gas or liquids. Since the design constraints are very different between gas and liquid tanks, they are treated separately here. First, we will deal with fuel tanks that contain liquid—namely petrol tanks—, and then with hydrogen storage tanks.

**Petrol tanks**

Usually, and this is the case, fuel tank is used to refer to the whole fuel storage system, i.e. the tank itself, the fuel pump, the fuel gauge, etc. Tanks are made of either plastic (HDPE) or steel; the other elements vary in composition. Here, we will model the whole system as if it were made entirely of steel. Thus, the mass of the system, including the fuel, is:

$$m_{ft} = m_{ft0} + m_f$$

where $m_{ft0}$ is the fuel tank without fuel and $m_f$ is the fuel mass. As the engine consumes fuel, the term $m_f$ varies, whilst the term $m_{ft0}$ remains constant. The variation of the fuel mass is given by the expression:

$$m_f(t) = m_{f0} - H_f \int_0^t \frac{P_m(t)}{\eta} dt$$

where $m_{f0}$ is the initial fuel's mass, $H_f$ is the fuel's heating value, $P_m$ is the engine power, and $\eta$ is the engine efficiency.

However, the mass of the fuel, even when the tank is full, is small compared to the total mass of the vehicle. For instance, the mass of a vehicle with an empty mass of 1000 kg and a tank capacity of 40 L only varies around 3% between empty and full tank. Therefore, it is not unwise to assume that the fuel tank mass is constant.

The mass of the fuel tank depends, basically, on its capacity. If we think of a tank as a sphere, then its capacity is proportional to its radius cubed, and the surface area of the metal sheet is proportional to the sphere's radius squared. If the tank has a constant thickness, then the mass of the tank is proportional to its surface area. This way, it is possible to estimate the tank's mass from its capacity.

$$V \sim r^3 \rightarrow r \sim V^{1/3} \tag{3.16}$$

$$S \sim r^2 \rightarrow S \sim V^{2/3} \tag{3.17}$$

$$m \sim S \rightarrow m = C \cdot V^{2/3} \tag{3.18}$$

The mass of the fuel tank of a typical passenger car is 54 kg [REF], and its capacity is 80 L [REF]. From the equation [eq], $C = 2.9$ kg/m$^2$.

The mass of the fuel depends on the volume and its density. The density of petrol is $\rho_{petrol} = 0.733$ kg/m$^3$. Then, the mass of the fuel tank, when full, is:

$$m_{ft} = \rho_{petrol} V + C V^{2/3}$$

**Hydrogen storage**

Hydrogen can be stored on-board as compressed gas, liquified, or as a metal hydride. Containing liquid hydrogen at cryogenic temperatures—13.95 K—is technically challenging, and metal hydrides require carrying a highly reactive hydride and a corrosive solution of hydroxide in the same vehicle. Hence, only compressed hydrogen is regarded here.

Hydrogen tanks are usually at 35 MPa (low pressure) or 70 MPa (high pressure). Since more pressure means more strength of the tank, both low and high pressure present similar specific energies. However, high pressure tanks have a better energy density, that is, require less space. For that reason, we will use a 70 MPa tank.

The hydrogen tank used is a basically a carbon fiber reinforced polymer vessel with an HDPE inner lining and a glass fiber outer lining. It also have a foam layer inside, and a balance-of-plant system, a set of components including pressure regulators, valves, etc. The hydrogen tank is sized from its energy capacity, based on [**?**]. Assuming a cylindrical vessel with semi spherical caps, the volume of the vessel is calculated. The next step is to estimate the thickness of the vessel required to withstand the pressure. Then, the masses of all layers are added to get the total system mass. Also, the energy requirements and emissions to manufacture the tank is calculated. The complete calculations can be found on [ANNEX].

# Chapter 4

# Preliminary design of the powertrain

In this chapter the sustainability of various powertrain configurations are analysed. In order to do so, simple models of the vehicles have been developed, and optimised using a genetic algorithm.

## 4.1 Vehicle specifications

Before designing, one must know the specifications of what is to be designed. Even though the aim is to find the most sustainable option, without restrictions, the vehicle has to be usable. Therefore, a set of minimum performance values must be specified. Also, we must define under which circumstances those values have to be measured.

### 4.1.1 Driving cycle

The powertrain response depends, basically, on three factors: the speed of the vehicle, its acceleration, and its history. Speed and acceleration determine the force that the powertrain must exert. Plus, the maximum force the powertrain can exert usually depends on the engine or motor speed, and hence on the vehicle speed. Lastly, some powertrain configurations vary their response according to the past speeds and accelerations. For instance, a the voltage of a battery decreases with the charge of the cells.

To assess the emissions and consumption of vehicles, vehicles are driven following a speed profile known as *driving cycle*. There are lots of standarised driving cycles. As part of the EU legislative driving cycles, the following driving cycles are of special interest for us.

**ECE-15**: urban driving cycle.

**EUDC**: extra-urban driving cycle.

**EUDC-low power**: extra-urban driving cycle for low power vehicles.

**NEDC**: New European Driving Cycle

The NEDC is the driving cycle used to measure the official emission and consumption figures given in the EU. It consists of four instances of the ECE-15, followed by one instance of the EUDC. This cycle was designed to model the usual operation of vehicles within Europe. Given that the vehicle we want to design is a urban vehicle, and as such will be low powered, the low power option for the extra-urban driving cycle seems more convenient. Since there is no NEDC for low power vehicles, we have copied the pattern of the NEDC but instead of the final EUDC, the EUDC-low power is used. The resulting driving cycle is that of [FIGURE] [1].

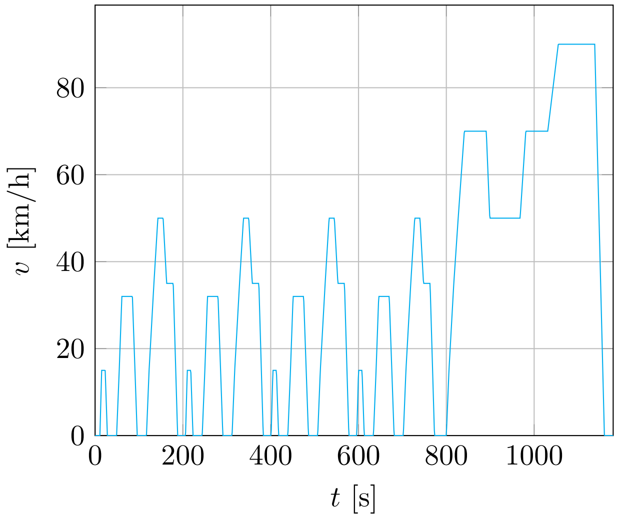


Figure 4.1: NEDC for low power vehicles

### 4.1.2 Acceleration time

Acceleration time is a very common performance parameter. Even though it does not say much about the general performance of a vehicle, it gives us an idea of its acceleration capability. It is usual to give the 0–100 km/h-acceleration times. However, we pretend to design an urban vehicle, so the acceleration time from still to 50 km/h is more convenient. In [**?**] the 0–30 mph[2] acceleration times of various electric vehicles are given. The car that takes more time to accelerate is the Prius PHEV, which in pure electric traction takes about 6 s. All the others take less than 4 s, so a maximum value of 5 s for our vehicle seems a good choice.

[1]The data points are available at[**?**]
[2]30 mph = 48.3 km/h which is a good a approximation

### 4.1.3 Maximum speed

Another common performance parameter is the maximum speed the vehicle can reach. It is assumed that the vehicle goes in a flat road and that when reaches the top speed, the acceleration is nil. Under those constraints, the vehicle dynamics' equation is:

$$F_t - F_{ae} - F_{rr} = 0 \rightarrow F_t = \frac{1}{2}\rho A_f C_d v^2 + f_r m g \tag{4.1}$$

This equation gives us the maximum speed the vehicle can sustain, but not the maximum speed the vehicle can reach. Since the tractive force is generally related to the vehicle speed and the transmission ratio, satisfying that equation does not guarantee the solution. Therefore, we will have to calculate the maximum speed with the numerical models.

Since sustainability—and not performance—is what we are looking for, designing a propulsion system to be able to reach the usual 200 km/h mark does not make sense. Plus, the maximum speed allowed in most countries is at most 120 km/h [FIGURE]. Therefore, a compromise value of 160 km/h seems reasonable.

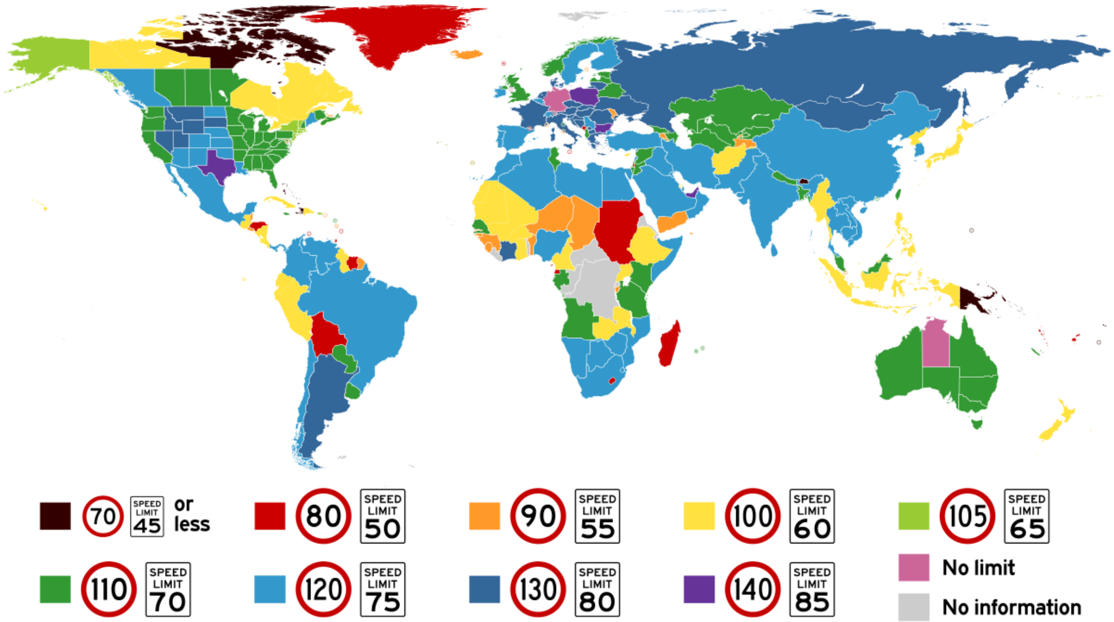


Figure 4.2: Highest posted speed limits. In km/h on the left and mph on the right [?]

### 4.1.4 Maximum slope

Uphills—and downhills—are usual in roads, so a vehicle must be able to overcome them. As shown in [TABLE]4.2, the maximum slope in an ordinary road is 18%, so climbing such a slope should be relatively easy. There are two ways of evaluating the hill climbing capabilities of a vehicle: the absolute maximum slope—at any speed—, and the maximum slope that the vehicle can climb at a certain speed. We will use the second, because it better describes real situations. The speed at which the vehicle must be able to climb the 18% slope is 50 km/h. The [EQUATION] must be solved in order to obtain the maximum slope that the vehicle can climb at that speed.

$$F_{t,max}(v) - \frac{1}{2}\rho A_f C_d v^2 - f_r mg\cos\alpha - mg\sin\alpha = 0 \tag{4.2}$$

### 4.1.5 Range

The range of a vehicle is the distance it can travel without needing recharging or refueling. Range is not a problem with internal combustion engine vehicles due to the high energy density of fuels, but with electric powered vehicles the issue of range arises. The fear that a vehicle has insufficient range to reach the destination has even a name—*range anxiety*—, but it is more of a psychological thing, fed by decades of driving hundreds of kilometers without needing to refuel, that an actual problem. In any way, electric vehicles do have less range than ICEV, so sizing the energy storage system is key in designing electric vehicles.

As we have seen in the section [SECTION], the majority of journeys from and to Barcelona are within a round-trip distance of around 100 km, so a range of 105 km is enough. Even in a longer distance trip, the vehicle can still be recharged—just as ICEV can be refueled—and there are more electric vehicle recharging stations available every day.

## 4.2 Models of the vehicles

### 4.2.1 Non-hybrid vehicles

The vast majority of vehicles today are non-hybrid—more precisely, internal combustion engine vehicles—. Including them in the analysis is a must, so that we have a frame of reference for comparing the results. The non-hybrid vehicles analysed are:

**ICEV**: Internal combustion engine vehicle

**BEV**: Battery electric vehicle

**FCV**: Fuel cell electric vehicle

### 4.2.2 Hybrid vehicles

Hybrid vehicles have better consumption figures, that non-hybrid. Although that comes at a cost of being more expensive—both economically and energetically—, the overall cost should be less than their non-hybrid counterparts. Here, two types of hybrid vehicles are analysed.

**HEV**: Hybrid electric vehicles

**HSEV** Hybrid storage electric vehicles

Hybrid electric vehicles are vehicles that have an ICE as a primary source of energy, and an electrical source of energy—usually a battery—capable of recovering braking energy. Although hybrid electric vehicle is a very vague term for referring to such vehicles, they are the most popular and the firsts to be on the market. The HEV that we have analysed has a petrol-fueled ICE and a Li-ion battery.

HSEV are purely electric vehicles that have a hybrid energy storage system. The reason for this is that some energy storage systems have good energy storage capabilities but poor power capabilities, and others the other way round. Then, combining them into a single energy storage system provides both good power and good energy capabilities whilst keeping the weight low. The combinations analysed are four:

- Fuel cell with ultracapacitors (FCUC)
- Fuel cell with flywheel (FCFW)
- Battery with ultracapacitors (BUC)
- Battery with flywheel (BFW)

## 4.3 Genetic algorithm

A genetic algorithm (GA) is a metaheuristic optimisation method inspired by natural selection. The process is very simple, but it can lead to high-quality solutions. The amount of non-linearities found in this particular optimisation problem, makes a genetic algorithm a good candidate.

The basic element of a genetic algorithm is the chromosome. A chromosome is a codified piece of information that can be evaluated by a fitness function. Each chromosome consists of a number of genes. For instance, in this context a gene could be the maximum power of the motor.

The basic constitution of the algorithm is:

1. Create a random population of chromosomes.
2. Evaluate each chromosome using a fitness function.
3. Select the fittest chromosomes according to their fitness value.
4. Combine the selected chromosomes performing the crossover operator.
5. Mutate a number of random genes.
6. Repeat until a satisfactory result is obtained.

A genetic algorithm has some advantages over others search algorithms. First, it travels the search space with more individuals, so it is less likely to get stuck in local optima. On the same direction, it uses *genotype*, rather than *phenotype* to travel that space—iėṪhe path is not changed through the visible characteristics of the individual, but through the genetic information that make those characteristics. Furthermore, the success of any optimisation algorithm relies on the proper balance between exploration and exploitation, that is to look over a wide space but also concentrating in good solutions. This balance is easily tuned in a GA through the mutation (exploration) and crossover (exploitation) rates.

### 4.3.1 Evaluation

The evaluation process in this particular case, consists of measuring the energy consumption of the vehicles through a simulation. Also, the manufacturing and assembly energy and emissions are calculated from the mass components of each vehicle. Since the vehicle needs to meet the specifications, the performance of the vehicle is evaluated as well. The process is as follows:

1. Extract the model parameters from the genetic information.
2. Simulate the vehicles under the driving cycle in order to get the consumption.
3. Evaluate the performance of the vehicle (performance coefficient).
4. Calculate the total energy burden and emissions (fitness value).
5. Correct the fitness value with the performance coefficient.

The performance parameters evaluated are: range—except in ICEV and HEV, since it is not an issue—, acceleration time from 0 to 50 km/h, maximum speed, and maximum slope at 50 km/h. Then, the parameters $p_p^i$ are averaged geometrically:

$$p_p = \left( \prod_i^N p_p^i \right)^{1/N} \tag{4.3}$$

After, a performance coefficient $p_c$ is calculated. This coefficient will correct the energy consumption, so that performance is also taken into account in the fitness evaluation. This function must meet the following requisites:

- It has to be neutral when the performance parameters equal the target parameters.
- It has to slightly reward better performers. The maximum reward is $MR_f$.
- It has to severely punish underperformers. The maximum punishment is $MP_f$.

The expression used is:

$$p_c = \frac{a}{p_p + b} + c \tag{4.4}$$

The parameters $a, b, c$ are fitted to satisfy the requirements. Thus,

$$c = MR_f \tag{4.5}$$

$$b = \frac{1 - MR_f}{MP_f - 1} \tag{4.6}$$

$$a = b\,(MP_f - MR_f) \tag{4.7}$$

### 4.3.2 Selection

To select the fittest chromosomes, a roulette-wheel can be used. First, it is necessary to compute the probability $P_i$ of being chosen of each chromosome $i$ from their fitness value $F_i$:

$$P_i = \frac{F_i}{\sum_i^N F_i} \tag{4.8}$$

Then, the cumulative probability $C_i$ of each chromosome can be calculated:

$$C_1 = P_1 \tag{4.9}$$

$$C_i = C_{i-1} + P_i \quad i = 2 \ldots N \tag{4.10}$$

The roulette-wheel is simulated generating as much random numbers $R_i$ as chromosomes are there. The random numbers must be between zero and one. If the random number $R_i$ is greater than the cumulative probability $C_j$, then the chromosome $j+1$ is the $i$-th chromosome selected. This process is repeated for each random number generated. It is worth noting that this process allows a chromosome to be selected more than once, which is what we want.

### 4.3.3 Crossover

Once the fittest chromosomes have been chosen, it is time to combine them. The process is similar to selection in that it involves generating random numbers. For each chromosome a random number is generated. If the random number $R_i$ for the chromosome $i$ is greater than the crossover rate $\rho_c$, the chromosome $i$ is selected as a parent. The crossover rate should be high so that good solutions produce offspring. Here, we have used a crossover rate of $\rho_c = 0.7$.

The selected parents are set to share their genes between them, but not with themselves—that would be useless. Simply translating each chromosome one place would do. For instance, if the chromosomes selected as parents are {1,3,6}, we translate each chromosome to the right, and the rightmost to the first place. This way we get {6,1,3}. Then chromosome 1 will mate with 6, 3 with 1, and 6 with 3.

Finally, the genes of each chromosome are interchanged between parents. The crossover point is the cutting point of the chromosome. It is a random integer between one and the number of genes minus one. The chromosomes that have not been selected as parents, are left as they are.

### 4.3.4 Mutation

In nature, some genes mutate spontaneously or due to external factors. Most of mutations are harmless, some of them are damaging, and few are beneficial. Those few beneficial mutations have led to us—even though it has taken millions of years—. That is why mutation is used.

The number of mutations is determined by the mutation rate $\rho_m$. First, we need to compute the total number of genes $N_g$, that is, the number of genes in a chromosome times the number of chromosomes in a population. Then, we generate a random integer $R_i$ between 1 and $N_g$ for each gene $i$ of the population. Then, if the random number generated for the gene $i$ is smaller than the product $\rho_m \cdot N_g$, then the gene $i$ is mutated. Mutating a gene consists of giving a new random value to that gene. Given the nature of the process, it is expected that the fraction of genes mutated will be near the mutation rate.

Unlike the crossover rate, the mutation rate should be small, since a high value would make good genes disappear. Here, a mutation rate of $\rho_m = 0.02$ is used.

## 4.4 Results

Once the algorithm is done, the values obtained are checked. First, of all the chromosomes in all populations for each type of vehicle, those that present simulation errors—due to lack of power or energy to complete the driving cycle—are eliminated. Then, the performance parameters are checked, so only the vehicles that meet the specifications are left. Of those vehicles, the best are listed in [TABLE].

The results presented in [TABLE] show that hybridisation is a good approach to minimize energy consumption, even if the energy involved in the whole life cycle of the vehicle is taken into account. Not only the figure of HEV is less than half of the ICEV, but also hybrid storage present incredible improvements. The two best options are, clearly, the battery hybrids, both with flywheel and ultracapacitors. Given that the results of the optimisation depend on the parameters used, it is not fair to say that ultracapacitors are a better option than flywheels.

However, given that our ultimate purpose is to design and implement the control system, a decision has to be made. Since there is a tie in the main parameter we were judging, we can take a look at the performance. The performance parameters of each vehicle is presented in [TABLE].

It is clear, then that the vehicle chosen is the Battery-Ultracapacitor Hybrid.

Table 4.1: Results of the GA after 1000 generations

| Vehicle | Corrected energy consumption [MJ/km] | Mass [kg] | Engine power [kW] | Motor power [kWh] | ESS1 capacity [kWh] | ESS2 capacity [kWh] |
|---|---|---|---|---|---|---|
| ICEV | 3.327 | 707 | 23.6 | – | – | |
| FCV | 1.245 | 658 | – | 36.0 | 73.4 | – |
| BEV | 1.236 | 880 | – | 41.5 | 10.7 | – |
| HEV | 1.342 | 790 | 10.6 | 32.9 | 11.9 | |
| FCFW | 1.103 | 714 | – | 41.8 | 33.7 | 5.2 |
| FCUC | 1.098 | 703 | – | 40.2 | 29.9 | 11.2 |
| BFW | 1.078 | 731 | – | 48.4 | 10.0 | 2.2 |
| BUC | 1.061 | 695 | – | 41.0 | 10.1 | 10.9 |

Table 4.2: Performance parameters of the best two vehicles

| Vehicle | BUC | BFW |
|---|---|---|
| Acceleration time [s] | 4.9 | 4.3 |
| Max speed [km/h] | 157 | 160 |
| Max grade at 50 km/h [%] | 25 | 25 |
| Range [km] | 146 | 110 |

# Chapter 5

# Final design and implementation of the control system

The design of the control system has been made with the Simulink software, using the macroscopic energy representation (MER). From the characteristics obtained in the previous section, a set of components have been chosen. In the following lines, each part of the control system is explained, the overall system is shown, and finally the results of the simulation are presented.

## 5.1 Elements of the system

In MER there are a set of symbols that represent the type of conversion. There are also blocks that represent the inversion of those conversions, so that the system can be controlled. In [FIGURE] we can see the blocks of EMR.

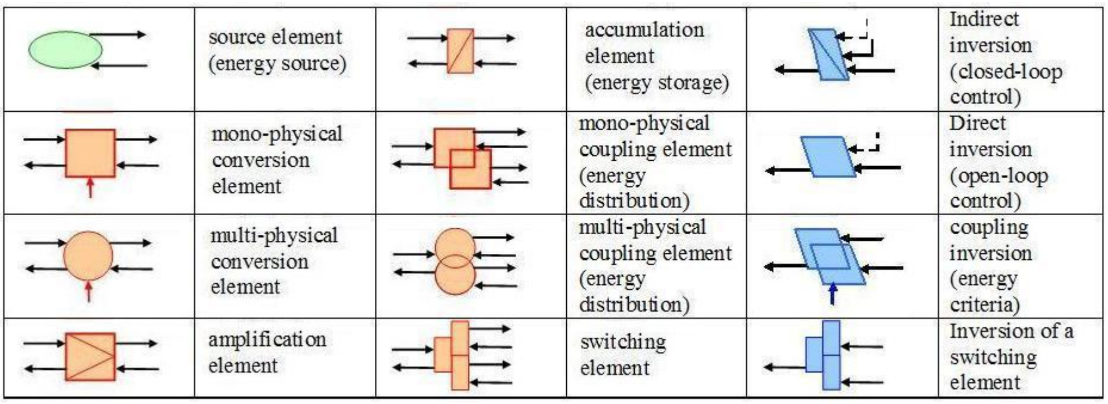


Figure 5.1: Blocks of the EMR

In the next lines the blocks comprising the system are described. Please note that the blocks are not ordered in the causality direction, but rather in groups which, in the eyes of the author, are more easily comprehensible.

### 5.1.1 Chassis, wheels, and environment

The environment is a source block. The input is the speed of the vehicle $v$ and the output is the resistive force $F_r$. The equations expressing their relationship are [EQUATIONS].

$$F_r = \frac{1}{2}\rho\, C_d\, A_f\, v^2 + f_r\, M\, g\, \cos(\alpha)\, \mathrm{sgn}(v) + M\, g\, \sin(\alpha) \tag{5.1}$$

The chassis represents the vehicle dynamic response. That is, given the force exerted by the motor and the force exerted by the environment, it gives the acceleration. The equation governing this block is [EQUATION]

$$v = \frac{1}{M}\int (F_t - F_r)\mathrm{d}t \tag{5.2}$$

Where $v$ is the resulting speed of the vehicle, $M$ is its mass, $F_t$ is the traction force, and $F_r$ is the resistive force.

Finally, the wheel is a mono-physical conversion element, which simply translates the linear variables into rotational variables and vice versa, through the wheel radius $R_w$.

$$F_t = \frac{\Gamma_w}{R_w} \tag{5.3}$$

$$v = \frac{\omega_w}{R_w} \tag{5.4}$$

### 5.1.2 Inverter, motor and transmission

The motor used is a surface-mounted permanent magnet synchronous motor (SPMSM), based on the motor of the CAT07e, the electric racing vehicle presented to Formula Student by the ETSEIB Motorsport team. The motor is a modified version of the MA-55 Mavilor motor, that can provide up to 42 kW of power [**?**].

The model of the motor consists of two blocks. First, the electromechanical conversion is a multi-physical conversion element, that converts electric power into mechanical power. The equation is [EQUATIONS]:

$$\Gamma_e = \frac{3\, n}{4}(\lambda_m\, i^r_{s,q} + (L_d - L_q)\, i^r_{s,d}\, i^r_{s,q} \tag{5.5}$$

Second, the winding losses represent the electric power that is not converted into mechanical power due to Joule effect or the magnetisation of the windings:

$$u_{s,d} = r_s\, i^r_{s,d} + L_d \frac{\mathrm{d}i^r_{s,d}}{\mathrm{d}t} - \omega_r\, L_q\, i^r_{s,q} \tag{5.6}$$

$$u_{s,q} = r_s\, i^r_{s,q} + L_q \frac{\mathrm{d}i^r_{s,q}}{\mathrm{d}t} + \omega_r\, L_d\, i^r_{s,d} + \omega_r\, \lambda_m \tag{5.7}$$

The model of the inverter used is a simple multiplication by the modulator signal $\alpha$. The losses of the inverter have not been included. The equations are:

$$u^r_{s,dq} = \alpha_{dq} \cdot U_{DC} \tag{5.8}$$

$$I_{DC} = \frac{3}{2} \langle \alpha_{dq}, i^r_{s,dq} \rangle \tag{5.9}$$

Finally, the transmission is a simple reduction to translate from motor variables to wheel variables.

$$\Gamma_w = \Gamma_m \, k_{red} \tag{5.10}$$

$$\omega_m = \omega_w \, k_{red} \tag{5.11}$$

### 5.1.3 Battery and ultracapacitors

The battery [EQUATION]and ultracapacitor [EQUATION] models are the same as described in the previous section [SECTION]. The battery imposes the DC bus voltage, and thus is connected directly to the DC bus coupler. The ultracapacitors, though, are connected through a DC converter and an inductive filter.

$$U_B = N_s^B \left[ \left( E_0 - K \frac{Q}{Q - \int \frac{I_B}{N_p^B} \mathrm{d}t} + A \, e^{-B \int \frac{I_B}{N_p^B} \mathrm{d}t} \right) - R_B \frac{I_B}{N_p^B} \right] \tag{5.12}$$

$$U_C = N s^C \left[ V_{C0} - \frac{1}{C} \int \left( \frac{I_C}{N_p^C} + \frac{V_C}{R_{leak}} \right) \mathrm{d}t - \frac{I_C}{N_p^C} R_C \right] \tag{5.13}$$

### 5.1.4 DC bus coupler, converter and filter

The DC bus coupler forces both the battery and the converter connected to the ultracapacitor to be at the same voltage. Also, distributes the current between them. The governing equations are:

$$U_{DC} = U_B = U_C^{conv} \tag{5.14}$$

$$I_B = I_{DC} - I_C^{conv} \tag{5.15}$$

The converter boosts the voltage of the ultracapacitor filter to meet the DC bus voltage. It is the same model of the inverter, but in direct current:

$$U_C^{conv} = \alpha_C \, U_{DC} \tag{5.16}$$

$$I_C^{conv} = \alpha_C \, I_C^{filter} \tag{5.17}$$

The filter between the ultracapacitors and the DC converter is a simple RL filter, that is, a series impedance consisting of a resistance and an inductance. The [EQUATION] shows that relation.

$$I_C = I_C^{conv} = \frac{1}{L_{filter}} \int \left( U_C - U_C^{conv} - R_{conv} \, I_C \right) \mathrm{d}t \tag{5.18}$$

### 5.1.5 Control elements

#### Inversion blocks

The inversion blocks perform the same operations of the blocks above described in the opposite direction. There are inversion blocks for the following elements: wheel, transmission, electromechanical conversion, winding losses, DC bus coupler, and DC converter.

#### Controllers

There are three controllers in this system: the speed loop, the current loop, and the ultracapacitor current controller. The ultracapacitor controller is a simple PI controllers, and the speed loop is just a P controller. The current loop, however, deserves more attention, since it has some elements that are very important for the control.

It is, indeed, a PI controller, but has three additional elements. First, there is a voltage saturation element that prevents the inverter from synthesising more voltage of which is capable[1]. However, if the voltage required by the PI is higher than allowed, the error will accumulate in the integrator, and the control will fail. For that reason, an anti-windup element has been added. It just measures the difference between the signal before saturation and the saturated signal and subtracts it before the integrator.

The other extraordinary element is the decoupler. As we can see in [EQUATIONS,del motor], the equations of both $q$ and $d$ axis are coupled, so it is impossible to control them separately. However, measuring the speed and the current it is possible to estimate the coupling effect and counteract it, so that we can control both currents separately.

#### Modulators

The modulators used here are simply an inversion of what takes place in the converters. For instance, the inverter multiplies the DC voltage by the modulator signal to get the $dq$ voltage. Then the modulator simply calculates this signal from the measured voltages.

$$\alpha_{dq} = \frac{u_{s,dq}^{r\star}}{U_{DC}} \tag{5.19}$$

$$\alpha_C = \frac{U_C^{conv\star}}{U_{DC}} \tag{5.20}$$

### 5.1.6 Strategy

The strategy block contains a fuzzy controller that tells the coupler inversion how much current it has to draw from the battery and the ultracapacitor.

Fuzzy logic is a very useful tool that allows for less restrictive states so that the operation is smoother. In boolean logic, there only exists two states: true or false, 1 or

[1]This element has been deactivated because it slowed down the simulation significantly. It does not change the results unless the signal to the inverter is actually higher than allowed.

0. In fuzzy logic, all the range from true to false, from 0 to 1 is allowed. It was first developed by Lotfi Zadeh [?] as an attempt to control machines just as humans do.

A fuzzy logic controller consists of three elements. First, the input membership functions (MF), tells the controller the state of a variable in broad terms. For instance, the value of the speed of the motor can be converted to *low, medium, high.* The MF say how much low, medium or high is the speed according to a distribution, and the state that has the highest value is adopted. Similarly, there are output membership functions that reverse that process in order to be usable in the control system. In the middle of those elements, there is a set of rules that relate the inputs and the outputs.

In this particular system, the input variables are the ultracapacitor state-of-energy (SoE), and the qualitative current required by the controller. The output variable is the current that has to be drawn or injected to the ultracapacitors.

The qualitative current is calculated as follows: from the DC current, the average value is computed with a certain frequency $f$. This average is the reference current. The actual current minus the reference current is the peak current. The idea is that the battery supply the reference current and the ultracapacitors the peak current. The value of the peak current is divided by a certain amount $I_{great}$ that represents how much deviation from the reference current is considered a great current. This value is saturated to [-1,1] and sent to the fuzzy controller, together with the other input variable—the SoE. The output variable is the UC current.

The MF of the fuzzy controller will discern wether the current is *below*, *similar*, or *above* the reference current. A similar process states if the SoE is *low* or high.

Then, the following set of rules are applied:

1. If current is *above* and SoE is *high* then *use* the UC.
2. If current is *above* and SoE is *low* then *don't use* the UC.
3. If current is *similar* then *don't use* the UC.
4. If current is *below* and SoE is *high* then *don't use* the UC.
5. If current is *below* and SoE is *low* then *use* the UC.

This simple set of rules, written in plain language, will command when the ultracapacitor is charged and discharged. Obviously it is probably not the most efficient way of doing it, but it is very simple, easy to implement and offers good results.

## 5.2 Overview of the system and results

The overall system is shown in [FIGURE]

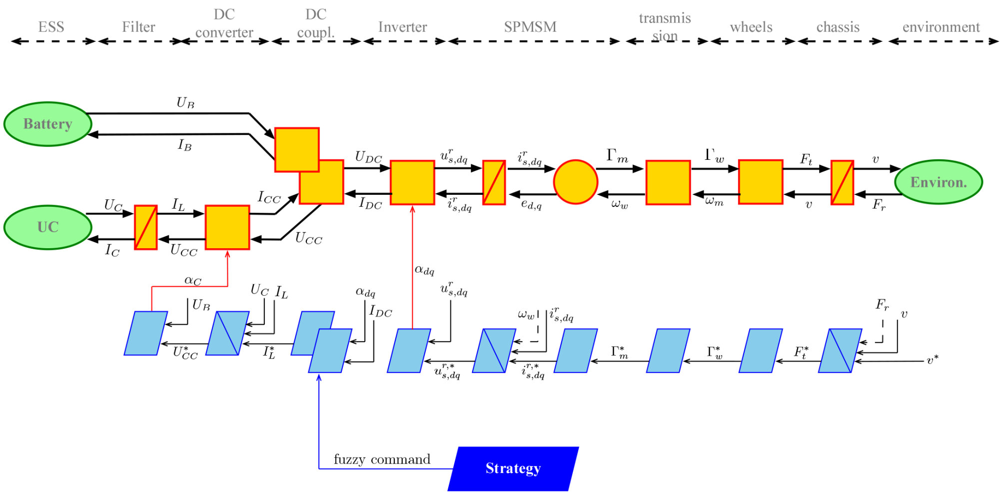


Figure 5.2: REM of the vehicle

The results of the control system are satisfactory. As we can see in [FIGURE], the vehicle follows perfectly the speed command. Looking at the current response, we can see that the fuzzy converter works well, since the ultracapacitor works in short bursts of high current, whilst the battery current is more stable, and has less abrupt changes.

The energy and emissions of operation are the only values that may change with respect to the preliminary design, because the components are the same. Then, measuring the operation energy and emissions is sufficient. The results are shown in [TABLE]. As we can see, the energy and emissions are slightly higher, but not significantly. The values obtained are still below those of all the other vehicles.

Table 5.1: Vehicle model parameters

| Symbol | Parameter | Units | Value |
|---|---|---|---|
| | **General parameters** | | |
| $\rho$ | Air density | $\mathrm{kg\,m^{-3}}$ | 1.22521 |
| $g$ | Acceleration of gravity | $\mathrm{m\,s^{-2}}$ | |
| $C_d$ | Drag coefficient | – | 0.3 |
| $A_f$ | Frontal area | $\mathrm{m^2}$ | 2.1 |
| $f_r$ | Rolling resistance coefficient | – | 0.0105 |
| $M$ | Vehicle mass | kg | 697 |
| $R_w$ | Wheel radius | m | 0.3 |
| $k_{red}$ | Transmission reduction | – | 4.24 |
| | **Motor parameters** | | |
| $P_m$ | Motor power | kW | 41 |
| $r_s$ | Winding resistance | $\Omega$ | 0.2 |
| $L_w$ | Winding inductance | mH | 1.9 |
| $n$ | number of pairs of poles | – | 2 |
| $L_d$,$L_q$ | Winding inductance in dq axis | mH | 1.3 |
| $\lambda_m$ | Flux linkage | $\mathrm{V\,s\,rad^{-1}}$ | 0.4832 |
| | **Battery parameters** | | |
| $Q$ | Charge | Ah | 1 |
| $E_0$ | Voltage constant | V | 3.7348 |
| $R_B$ | Internal resistance | $\Omega$ | 0.09 |
| $K$ | Polarisation voltage | V | $8.76\,10^{-3}$ |
| $A$ | Voltage drop of exponential zone | V | 0.468 |
| $B$ | 3/Charge at the end of exponential zone | $(\mathrm{Ah})^{-1}$ | 3.5294 |
| | **Ultracapacitor parameters** | | |
| $C$ | Capacitance | F | 3500 |
| $V_{C0}$ | Initial voltage | V | 2.85 |

Table 5.2: Comparison of the results with the preliminary version

| Parameter | Preliminary design | Final design |
|---|---|---|
| Energy of operation [MJ/km] | 0.4383 | 1.0609 |
| Total corrected energy [MJ/km] | 0.4553 | 1.0782 |

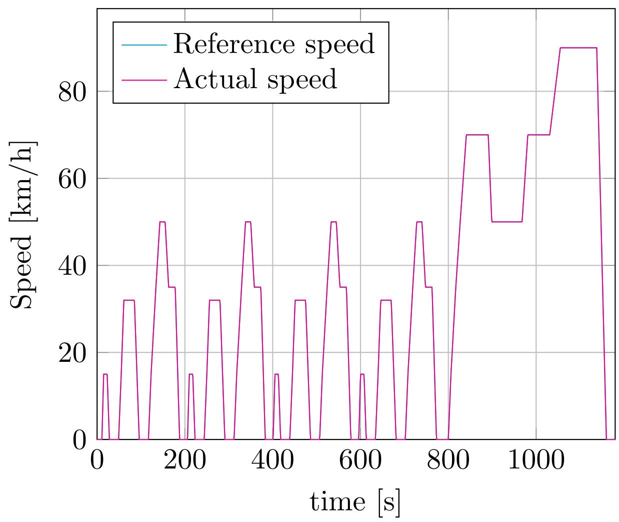


Figure 5.3: Speed profile

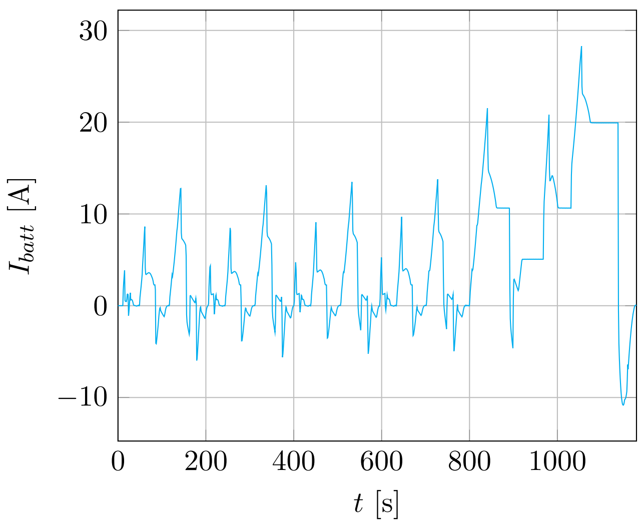


Figure 5.4: Battery current

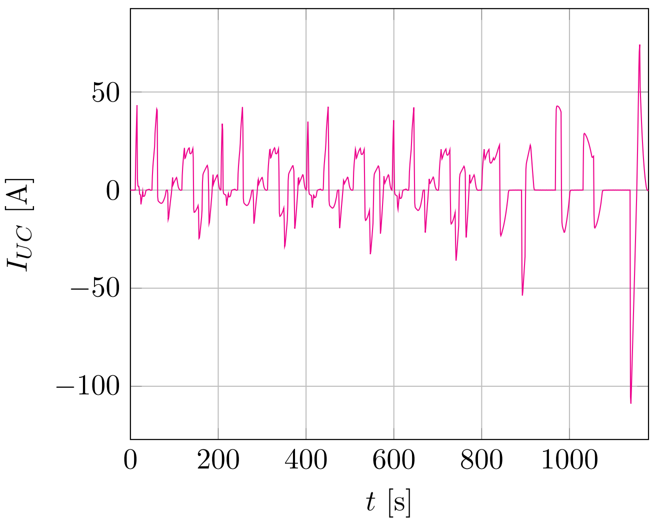


Figure 5.5: Ultracapacitors current

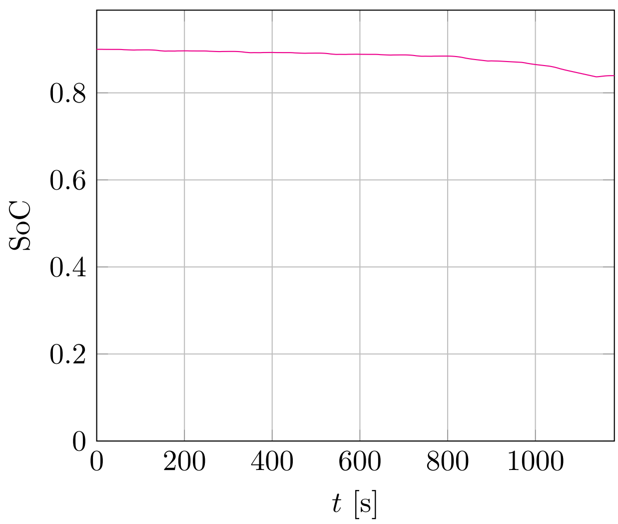


Figure 5.6: Battery state-of-charge

# Chapter 6

# Environmental impact

The environmental impact of this vehicle depends, besides the vehicle, on the conditions the vehicle is used. For this reason, different scenarios are presented.

On the one hand, three different occupation factors are considered: 1.2 (current), 1.5, and 2. On the other hand, three different substitution rates are considered, too: 10%, 50%, and 100%.

The vehicle used as a reference is the best ICEV found in [CHAPTER]. Even though it does not represent the real cars in the city, using it will manifest the improvement over ICEV, even if those are designed to be thrifty. [TABLE] shows the depletion of non-renewable resources and emissions of both vehicles, as well as the corrected energy values.

Table 6.1: Depletion and emissions of the vehicles

| Vehicle | Depletion [MJ/km] | Emissions [kg$CO_2$e/km] | Corrected energy [MJ/km] |
|---|---|---|---|
| ICEV (reference) | 3.272 | 0.2367 | 3.327 |
| BUC (designed) | 1.060 | 0.0767 | 1.078 |

The mean private transport journey time is $\bar{t}25.44\,\mathrm{min}$, and the mean speed is $\bar{v} = 21\,\mathrm{km/h}$ [**?**]. Therefore, the mean distance that a car travels is $\bar{d} = 8.9\,\mathrm{km}$.

$$\bar{d} = \bar{v}\,\bar{t} \tag{6.1}$$

From this figure and the number of circulating cars $N_c(t)$ for each occupation factor $f_o$ found in [SECTION], we can calculate the daily emissions and depletion due to private transport in the city of Barcelona. The daily vehicle-km travelled can be calculated with [EQUATION].

$$d_v = \bar{d} \int N_c(t)\mathrm{d}t \tag{6.2}$$

Table 6.2: Daily vehicle-km travelled for each occupation factor

| $f_o$ | $d_v$ [veh·km] |
|---|---|
| 1.2 | 7782.2 |
| 1.5 | 6222.9 |
| 2 | 4667.2 |

The base case is the current scenario, with an occupation factor of $f_o = 1.2$ and a substitution factor of $s_f = 0$. The depletion of non-renewable resources is $D = 25.46\,\mathrm{GJ}$ daily and the GHG emissions are $G = 1.842\,\mathrm{tCO_2e}$ daily.

The following tables [TABLE and TABLE] show the values for each scenario presented, and the difference with respect the base case (between parentheses).

Table 6.3: Depletion of non-renewable resources and emissions improvement

| Depletion [GJ] (improvement [%]) | | | |
|---|---|---|---|
| | $s_f = 0.1$ | $s_f = 0.5$ | $s_f = 1$ |
| $f_o = 1.2$ | 23.74 (-6.7) | 16.86 (-33.8) | 8.25 (-67.6) |
| $f_o = 1.5$ | 18.97 (-25.4) | 13.48 (-47.1) | 6.59 (-74.1) |
| $f_o = 2$ | 14.24 (-44.1) | 10.11 (-60.3) | 4.95 (-80.6) |
| Emissions [$tCO_2e$] (improvement [%]) | | | |
| $f_o = 1.2$ | 1.72 (-6.8) | 1.22 (-33.8) | 0.60 (-67.6) |
| $f_o = 1.5$ | 1.37 (-25.4) | 0.98 (-47.1) | 0.48 (-74.1) |
| $f_o = 2$ | 1.03 (-44.1) | 0.73 (-60.3) | 0.36 (-80.6) |

The improvements are pretty impressive, taking bearing in mind that the reference vehicle is more ecological than the real cars in the city.

# Conclusions

The results have shown that an improvement in the powertrain efficiency, is beneficial to the overall consumption of a city's transport system. However, it is clear that other measures regarding private transport are decisive too. For instance, increasing the occupation factor of the vehicles reduces the number of vehicles necessary, and thus the need no manufacture so many cars.

In the scope of the energetic system, we have seen that even though the energy coming from fossil fuels will decrease in the future, renewables can sustain a relatively high energy consumption. However, the energy consumption cannot increase indefinitely. Hence, it is necessary to rethink our transport system, as well as the economic system.

# Bibliography

[1] R. U. Ayres. The second law, the fourth law, recycling and limits to growth. *Ecological Economics*, 29(3):473–483, 1999.

[2] R. Bott. Lightweight Materials for Automotive Application. *Igarss 2014*, (1):29, 2014.

[3] A. Burnham. Updated Vehicle Specifications in the GREET Vehicle-Cycle Model. (July):1–40, 2012.

[4] A. Cobert. Environmental Comparison of Michelin Tweel and Pneumatic Tire Using Life Cycle Analysis Approved. (December), 2009.

[5] I. d. R. i. M. de Barcelona. Enquesta de Mobilitat Quotidiana de Catalunya. EMQ 2006. Principals resultats. pages 1–78, 2007.

[6] IEA-GIA. Trends in Geothermal Applicatons. page 42, 2010.

[7] Ipcc. Summary for Policymakers: Emissions Scenarios. A Special Report of Working Group III of the Intergovernmental Panel on Climate Change. *Group*, page 20, 2000.

[8] G. Keoleian, S. Miller, R. D. Kleine, A. Fang, and J. Mosley. Life Cycle Material Data Update for GREET Model. page 214, 2012.

[9] J. Laherrere. Oil and gas : what future ? *Groningen annual Energy Convention 21 November 2006*, (November):31, 2006.

[10] D. Montesinos-Miracle, C. Fontán-Tebar, and H. Vidal-Salvia. Simulation of an electric racing car using energetic macroscopic representation. *2014 IEEE Vehicle Power and Propulsion Conference, VPPC 2014*, 2015.

[11] S. Papasavva, S. Kia, J. Claya, and R. Gunthert. Life Cycle Environmental Assessment of Paint Processes. 74(925), 2002.

[12] PE International. Life Cycle Assessment of Cotton Fiber & Fabric Full Report. page 156, 2012.

[13] J. G. Speight. *The Chemistry and Technology of Petroleum - 5th ed.* 2007.

[14] O. Tremblay, L.-a. Dessaint, and a. I. Dekkiche. A Generic Battery Model for the Dynamic Simulation of Hybrid Electric Vehicles. *2007 IEEE Vehicle Power and Propulsion Conference*, (V):284–289, 2007.

[15] B. Vanni, G. L. Baldo, and J. Legarth. LCA Approach to the Automotive Glass Recycling. (November):1–32, 1995.

# Appendix A

# Combustion emissions

## A.1 Data

NOTE: The figures above are based on LHV.

## A.2 Assumptions

- Other pollutants emissions are negligible in terms of global warming potential.
- A consumption of 5 L/100km consumption of a petrol-fueled vehicle is assumed to calculate specific emissions for $N_2O$ and $CH_4$.
- The share of each type of coal that is burned remains constant overtime.

## A.3 Calculations

Emissions of carbon dioxide equivalent are calculated as follows:

$$e_{\mathrm{CO_2}e} = \sum e_i \cdot \mathrm{GWP}_i$$

The emission factors of mobile combustion for methane and nitrogen oxide must be converted to kg/mmBtu. To do so, we will use a conversion factor:

$$\frac{5\ \mathrm{L}}{100\ \mathrm{km}} \frac{1\ \mathrm{gal}}{3.79\ \mathrm{L}} \frac{0.125\ \mathrm{mmBtu}}{1\ \mathrm{gal}} \frac{1.609\ \mathrm{km}}{1\ \mathrm{mi}} = 2.653 \cdot 10^{-3}\ \mathrm{mmBtu/mi}$$

The emission factors for freight transportations are given in ton-miles. To convert them to tonne-kilometre, a conversion factor of 1 ton-mile= 1.460 t-km is used. To convert between values based on HHV to LHV:

$$e_{\mathrm{LHV}} = e_{\mathrm{HHV}} \frac{\mathrm{HHV}}{\mathrm{LHV}}$$

And, finally, a conversion factor of 1 mmBtu= 1.055 GJ is used.

Table A.1: Combustion emission factors (source: 1)

| Stationary combustion emission factors | | | |
|---|---|---|---|
| Fuel | $CO_2$ [kg/mmBtu] | $CH_4$ [g/mmBtu] | $N_2O$ [g/mmBtu] |
| Coal | | | |
| Mixed[1] | 95.52 | 11 | 1.6 |
| Anthracite | 103.69 | 11 | 1.6 |
| Bituminous | 93.28 | 11 | 1.6 |
| Sub-bituminous | 97.17 | 11 | 1.6 |
| Lignite | 97.72 | 11 | 1.6 |
| Petroleum | | | |
| Crude oil | 74.54 | 3.0 | 0.60 |
| Fuel Oil 5 | 72.93 | 3.0 | 0.60 |
| Fuel Oil 6 | 75.10 | 3.0 | 0.60 |
| Natural gas | 53.06 | 1.0 | 0.10 |
| Mobile combustion emission factors | | | |
| Fuel | $CO_2$ [kg/gal] | $CH_4$ [g/mi] | $N_2O$ [g/mi] |
| Petrol | 8.78 | 0.0173 | 0.0036 |
| Ethanol | 5.75 | 0.0550 | 0.0670 |
| Diesel (constr.)[2] | 10.21 | 0.57 | 0.26 |
| Product transport emission factors | | | |
| Vehicle | $CO_2$ kg/ton-mile | $CH_4$ g/ton-mile | $N_2O$ g/ton-mile |
| Waterborne craft | 0.042 | 0.0004 | 0.0027 |

[1]Mixed (Electric Power Sector)

[2]$CH_4$ and $N_2O$ figures in g/gal

## A.4 Results

### A.4.1 General emissions

### A.4.2 Stationary combustion (power sector)

### A.4.3 Marine freight transportation fuel

### A.4.4 Passenger transportation fuels

## A.5 Sources

1. Emission Factors for Greenhouse Gas Inventories.

2. Intergovernmental Panel on Climate Change (IPCC), Fourth Assessment Report (AR4), 2007.

Table A.2: Global warming potential factors (source: 2)

| Gas | 100-year GWP factor |
|---|---|
| $CH_4$ | 25 |
| $N_2O$ | 298 |

Table A.3: Share of each type of coal

| Coal | Share[%] |
|---|---|
| Anthracite | 1 |
| Bituminous | 52 |
| Sub-bituminous | 30 |
| Lignite | 17 |

3. Biomass Energy Data Book–2011

Table A.4: Heating values(source: 3)

| Fuel | LHV [MJ/kg] | HHV [MJ/kg] | HHV/LHV |
|---|---|---|---|
| Coal | 22.732 | 23.968 | 1.054 |
| Crude oil | 42.686 | 45.543 | 1.067 |
| Conventional gasoline | 43.448 | 46.536 | 1.071 |
| US conventional diesel | 42.791 | 45.766 | 1.070 |
| Residual oil | 39.466 | 42.21 | 1.070 |
| Natural gas | 47.141 | 52.225 | 1.108 |

Table A.5: General emissions of fossil fuels

| Resource | $CO_2$ [kg/mmBtu] | $CH_4$ [g/mmBtu] | $N_2O$ [g/mmBtu] | $CO_2e$ [kg/GJ HHV] | $CO_2e$ [kg/GJ LHV] |
|---|---|---|---|---|---|
| Coal[1] | 95.31 | 11.00 | 1.60 | 91.05 | 96.00 |
| Oil | 74.54 | 3.00 | 0.60 | 70.89 | 75.81 |
| Gas | 53.06 | 1.00 | 0.10 | 50.35 | 55.78 |

[1]Weighted average of the four types of coal

Table A.6: Stationary combustion emissions (power sector)

| Fuel | $CO_2$ [kg/mmBtu] | $CH_4$ [g/mmBtu] | $N_2O$ [g/mmBtu] | $CO_2e$ [kg/GJ HHV] | $CO_2e$ [kg/GJ LHV] |
|---|---|---|---|---|---|
| Coal | 95.52 | 11.00 | 1.60 | 91.25 | 96.21 |
| Oil[1] | 74.02 | 3.00 | 0.60 | 70.40 | 75.27 |
| Gas | 53.06 | 1.00 | 0.10 | 50.35 | 55.78 |

[1]Average of fuel oil 5 and 6

Table A.7: Marine freight transportation

| Vehicle | $CO_2$ [kg/ton-mile] | $CH_4$ [g/ton-mile] | $N_2O$ [g/ton-mile] | $CO_2e$ [kg/ton-mi] | $CO_2e$ [kg/t-km] |
|---|---|---|---|---|---|
| Waterborne craft | 0.042 | 0.0004 | 0.0027 | 0.043 | 0.029 |

Table A.8: Residual oil characteristics

| Parameter | Value | Units |
|---|---|---|
| $CO_2$ emission factor | 11.27 | kg/gal |
| Density | 3.752 | kg/gal |
| LHV | 39.466 | MJ/kg |

Table A.9: Passenger transportation fuel emissions

| Fuel | $CO_2$ [kg/gal] | $CH_4$ [g/mi] | $N_2O$ [g/mi] | $CO_2e$ [kg/GJ LHV] |
|---|---|---|---|---|
| Petrol | 8.78 | 0.0173 | 0.0036 | 72.23 |
| Ethanol | 5.75 | 0.055 | 0.067 | 79.03 |
| Ethanol[1] | 0 | 0.055 | 0.067 | 7.62 |

[1]Substracting the direct $CO_2$ emitted

# Appendix B

# Nuclear energy

## B.1 Nuclear electricity production

[FIGURE] shows nuclear electricity production $E(t)$ from 2006 to 2012 [1] and forecasts from 2020 to 2040 [2].

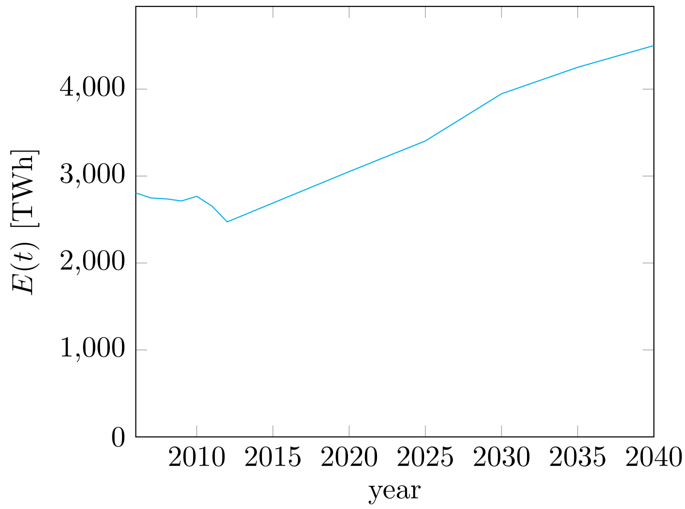


Figure B.1: Nuclear electricity production data and forecasts

From this data we calculate the cumulative electricity production $E_c$ from 2006:

$$E_c(t) = \int_{2006}^{t} E(\tau)\,\mathrm{d}\tau \tag{B.1}$$

## B.2 Uranium consumption by the reference reactor

[TABLE] presents the parameters of the reference reactor [3].

Table B.1: default

| Parameter | Symbol | Units | Value |
|---|---|---|---|
| First core natural U mass | $m_{fc}$ | Mg | 503.6 |
| Reload natural U mass | $m_r$ | Mg | 162.35 |
| Reload periods | $N_r$ | – | 30 |
| Lifetime | $t_{lt}$ | FPY[1] | 24.6 |
| Power | $P$ | GW | 1 |

[1]FPY = Full Power Years

The uranium consumed over the lifetime is:

$$m_{lt} = m_{fc} + (N_r - 1)\, m_r = 5211.8\,\mathrm{Mg} \tag{B.2}$$

The electricity produced over the lifetime is:

$$E_{lt} = P\, t_{lt} = 215.5\,\mathrm{TWh} \tag{B.3}$$

From those values, the uranium consumption of nuclear reactors can be deduced:

$$c_U = \frac{m_{lt}}{E_{lt}} = 24.18\,\mathrm{Mg/TWh} \tag{B.4}$$

With that value, and the cumulative electricity production from 2006, the cumulative uranium consumption from 2006 is obtained:

$$M_U(t) = c_U\, E_c(t) \tag{B.5}$$

## B.3 Uranium ore grade

The reserves of uranium by grade are taken from [3]. The cumulative amount of uranium by ore grade tells us how uranium of a minimum ore grade is there [FIGURE]. The blue dot represents the state of uranium resources in 2020, and the red dot in 2040.

Since the profitability of nuclear energy depends on the uranium ore grade, we can calculate the energy inputs up to 2020 and 2040, the electricity produced and estimate an average during this period. The energy input is calculated with the process described in [3], and the electricity is already calculated.

## B.4 Emission and depletion factors

During this period, we find that the total energy input to nuclear power is $E_i = 1.359\,10^{20}$ J, and the total electricity produced is $E_o = 7.405\,10^4$ TWh. Then, the average EROI (wire) is $EROI = 1.961$. The equivalent primary energy EROI—more convenient to compare with other energy sources—is $EROI_{pr} = 5.160$. With a depletion factor of

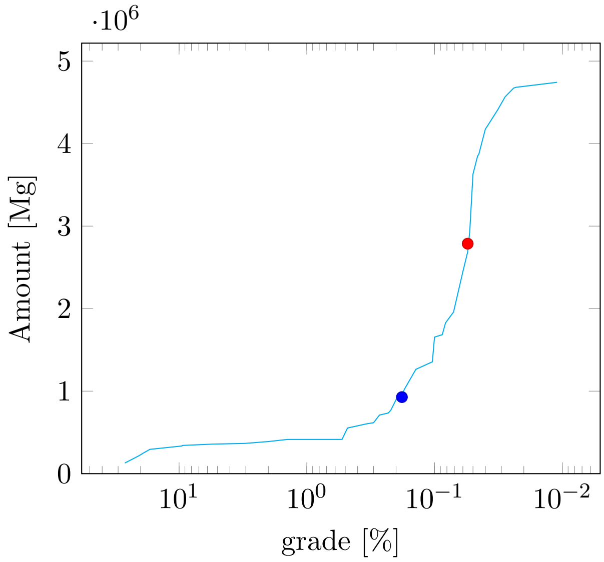


Figure B.2: Amount of uranium by minimum ore grade

$d_{in} = 0.959$ and an emission factor of $g_{in} = 71.30\,\mathrm{kgCO_2e/GJ}$ for energy inputs, the depletion factor and emission factor of nuclear energy in this period is:

$$d = 1 + d_{in}\, EROI_{pr}^{-1} = 1.186 \tag{B.6}$$

$$g = g_{in}\, EROI_{pr}^{-1} = 13.84\,\mathrm{kgCO_2e/GJ} \tag{B.7}$$

## B.5 References

[1] *BP Statistical Review June 2016*, 2016

[2] *International Energy Outlook 2016*, 2016

[3] Storm van Leeuwen, J.W, *Nuclear Power Insights*, 2012.

# Appendix C

# Corn ethanol

## C.1 Data

Table C.1: Corn ethanol characteristics

| | Units | Value |
|---|---|---|
| Ethanol LHV | MJ/kg | 26.95 |
| Ethanol density | $g/cm^3$ | 0.789 |
| Maximum stover yield | t/ha | 2.2 |
| Ethanol yield (stover) | L/t | 340 |
| Energy input (stover) | MJ/L | 5.8 |
| Grain yield | t/ha | 8.2 |
| Ethanol yield (grain) | L/t | 380 |
| Energy input (grain) | MJ/L | 22.4 |

## C.2 Combustion

Combustion emissions of ethanol are 7.62 kg $CO_2$e/GJ (source: 1).

## C.3 Obtention

One hectare of land yields 8.2 t of corn grain and 2.19 t of corn stover. With that we can obtain

$$V_{E,grain} = 8.2 \text{ t} \cdot 380 \text{ L t}^{-1} = 3116.0 \text{ L}$$
$$V_{E,stover} = 2.2 \text{ t} \cdot 340 \text{ L t}^{-1} = 744.6 \text{ L}$$

The total volume of ethanol is

$$V_E = V_{E,grain} + V_{E,stover} = 3860.6 \text{ L}$$

Then, the weighted mean energy input is

$$E_{input} = \frac{1}{V_E} \cdot (E_{i,grain} V_{E,grain} + E_{i,stover} V_{E,stover}) = 19.20 \text{ MJ/L}$$

Finally, the energy input to energy output ratio, $r_{i/o}$, is

$$r_E = \frac{E_{input}}{\text{LHV}_{ethanol} \cdot \rho_{ehtanol}} = 0.903$$

With a depletion factor of $d_{input} = 0.959$ and an emission factor of $e_{input} = 71.39$ kg $CO_2$e/GJ, we have a depletion factor of corn ethanol of $d_{ethanol} = 0.866$, and upstream emissions of 64.47 kg $CO_2$e/GJ.

## C.4 Results

Table C.2: Corn ethanol depletion and emission factors

| Fuel | Upstream emissions [kg $CO_2$e/GJ] | Combustion emissions [kg $CO_2$e/GJ] | Total emissions [kg $CO_2$e/GJ] | Depletion factor [GJ/GJ] |
|---|---|---|---|---|
| Corn ethanol | 64.47 | 7.62 | 72.09 | 0.866 |

## C.5 References

1. Annex: Estimation of fuel combustion emission factors.

# Appendix D

# Electricity

## D.1 Data

Table D.1: Electricity production by source [PWh] (source: 1)

| Source | 2020 | 2025 | 2030 | 2035 | 2040 |
|---|---|---|---|---|---|
| Petroleum | 0.86 | 0.69 | 0.62 | 0.59 | 0.56 |
| Nuclear | 3.05 | 3.40 | 3.95 | 4.25 | 4.50 |
| Natural gas | 5.26 | 6.30 | 7.47 | 8.78 | 10.14 |
| Coal | 9.73 | 10.07 | 10.12 | 10.31 | 10.62 |
| Renewables | 6.87 | 7.89 | 8.68 | 9.64 | 10.63 |

Table D.2: Renewable electricity from models [GW] (source: 2)

| Source | 2020 | 2025 | 2030 | 2035 | 2040 |
|---|---|---|---|---|---|
| Wind | 323.34 | 858.94 | 1994.34 | 3843.77 | 5864.27 |
| Solar (thermal) | 7.12 | 27.72 | 106.59 | 391.99 | 1245.14 |
| Solar (PV) | 296.18 | 721.91 | 921.13 | 963.24 | 970.33 |
| Hydro | 474.34 | 517.11 | 559.63 | 601.30 | 641.55 |
| Geothermal | 11.06 | 13.11 | 15.52 | 18.35 | 21.69 |

## D.2 Calculations

The share of each source within the period 2020–2040 is calculated as follows:

$$s_i = \frac{\int_{2020}^{2040} P_i \mathrm{d}t}{\sum_j \int_{2020}^{2040} P_j \mathrm{d}t}$$

With an electric distribution efficiency of 92% for all sources—world average losses were 8.16% in 2013 (source: 3)—, a thermal efficiency of 38% for petroleum, nuclear, and

Table D.3: Depletion and emission factors (source: 2)

| Source | Depletion factor | Emission factor [kg $CO_2$e/GJ] | Plant COM[1] [GJ/GJ] |
|---|---|---|---|
| petroleum | 1.250 | 95.35 | 0.084 |
| nuclear | 1.186 | 13.84 | - |
| gas | 1.213 | 86.87 | 0.030 |
| coal | 1.167 | 112.14 | 0.031 |
| wind | 0.053 | 3.97 | - |
| solar (thermal) | 0.548 | 40.79 | - |
| solar (PV) | 0.107 | 7.93 | - |
| hydro | 0.011 | 0.85 | - |
| geothermal | 0.107 | 7.93 | - |

[1]Plant construction, operation, and maintenance cost (- indicates that it is already included in the depletion and emission factors).

coal plants, and a thermal efficiency of 55% for gas plants, the depletion and emission factors are calculated.

$$d_e = \sum_{j=1}^{N} d_j \cdot s_j \cdot \eta_e^{-1} \cdot \eta_j^{-1} + s_j \cdot \eta_e^{-1} \cdot C_{\mathrm{COM}} \cdot d_{\mathrm{COM}}$$

$$e_e = \sum_{j=1}^{N} e_j \cdot s_j \cdot \eta_e^{-1} \cdot \eta_j^{-1} + s_j \cdot \eta_e^{-1} \cdot C_{\mathrm{COM}} \cdot e_{\mathrm{COM}}$$

## D.3 Results

Table D.4: Electricity depletion and emission factors

| Source | Depletion | Emissions [kg $CO_2$e/GJ] |
|---|---|---|
| petroleum | 0.077 | 5.88 |
| nuclear | 0.421 | 4.91 |
| gas | 0.593 | 42.50 |
| coal | 1.107 | 106.13 |
| wind | 0.010 | 0.71 |
| solar (thermal) | 0.010 | 0.71 |
| solar (PV) | 0.007 | 0.51 |
| hydro | 0.000 | 0.04 |
| geothermal | 0.000 | 0.01 |
| TOTAL | 2.225 | 161.40 |

## D.4 References

1. International Energy Outlook 2016.

2. Own models

3. http://data.worldbank.org/indicator/EG.ELC.LOSS.ZS

# Appendix E

# Energy inputs to the energy sector

## E.1 Data

Table E.1: Electricity production by source [PWh] (source: 1)

| Source | 2020 | 2025 | 2030 | 2035 | 2040 |
|---|---|---|---|---|---|
| Petroleum | 0.86 | 0.69 | 0.62 | 0.59 | 0.56 |
| Nuclear | 3.05 | 3.40 | 3.95 | 4.25 | 4.50 |
| Natural gas | 5.26 | 6.30 | 7.47 | 8.78 | 10.14 |
| Coal | 9.73 | 10.07 | 10.12 | 10.31 | 10.62 |
| Renewables | 6.87 | 7.89 | 8.68 | 9.64 | 10.63 |

Table E.2: Energy delivered to industrial sector by source [quad] (source: 1)

| Source | 2020 | 2025 | 2030 | 2035 | 2040 |
|---|---|---|---|---|---|
| Liquids | 72.18 | 76.52 | 80.59 | 84.61 | 88.59 |
| Natural Gas | 56.25 | 62.02 | 68.01 | 74.51 | 80.39 |
| Coal | 62.03 | 64.33 | 66.00 | 67.51 | 68.70 |
| Electricity | 37.16 | 39.97 | 42.16 | 44.32 | 46.31 |
| Renewables | 18.22 | 19.74 | 21.26 | 23.03 | 25.07 |

## E.2 Calculations

Using trapezoidal integration, we calculate the amount of electricity produced by source in the period. Then, we calculate the direct depletion of non-renewable resources by multiplying each share by the inverse of its power plant efficiency—1/38% for petroleum, nuclear, and coal; 1/55% for natural gas; and 0 for renewables—. In a similar fashion, we calculate the emissions of each source as the product of the direct emission factor and the depletion. The results are listed in table 3.

Table E.3: Electricity direct emissions and depletion

| Source | Total electricity [PWh] | Share [%] | Depletion | Emissions [kg $CO_2$e/GJ] |
|---|---|---|---|---|
| Petroleum | 13.05 | 2.11 | 0.055 | 4.17 |
| Nuclear | 76.88 | 12.41 | 0.327 | 0.00 |
| Natural gas | 151.25 | 24.42 | 0.444 | 24.77 |
| Coal | 203.38 | 32.84 | 0.864 | 82.96 |
| Renewables | 174.80 | 28.22 | 0.000 | 0.00 |
| TOTAL | | | 1.690 | 111.90 |

The total energy input to industrial sector depletion and emission factors are calculated in the same way. First, we calculate the share of each source. Electricity must be corrected, because the values given are the primary energy equivalent. Then, we multiply each share for a direct depletion factor—1 for fossil fuels, the value obtained before for electricity, and 0 for renewables. The sum of these values is the depletion factor. Similarly, multiplying each share for its emission factor and adding up the results, gives us the emission factor. It should be noted that the liquids figure includes, apart from oil products, fuels from other sources, such as biofuels. However, and given that the most part of it is oil, we will treat it as if it were solely oil.

Table E.4: Energy input to industrial sector emission and depletion factors

| Source | Total production[1] [quad] | Share [%] | Depletion | Emissions [kg $CO_2$e/GJ] |
|---|---|---|---|---|
| Liquids | 1522.70 | 31.98 | 0.320 | 24.07 |
| Natural gas | 1285.08 | 26.99 | 0.270 | 15.06 |
| Coal | 1247.45 | 26.20 | 0.262 | 25.15 |
| Electricity | 302.22 | 6.35 | 0.107 | 7.10 |
| Renewables | 403.25 | 8.47 | 0.000 | 0.00 |
| TOTAL | | | 0.959 | 71.39 |

[1] Electricity total production has been multiplied by a factor of 0.38 to undo the primary energy correction

## E.3 References

1. International Energy Outlook 2016.

# Appendix F

# Hydrogen storage

### Data and assumptions

Data from [1]

- The pressure tank is a cylindrical vessel with semi-spheric caps.
- The structural material is CFRP. It has an inner lining of HDPE and an outer lining of GF.
- There is a foam layer at both caps which is assumed to be the same size, regardless of the tank capacity.
- Balance-of-plant (BOP) is a set of components that include pressure regulators, valves, etc. It is also assumed to have a constant weight.
- $H_2$ is assumed to behave as an ideal gas.

| Parameter | Value |
|---|---|
| Inner lining thickness | 5 mm |
| Outter lining thickness | 1 mm |
| L/D | 3 |
| Nominal pressure | 35 MPa |
| Empty pressure | 20 MPa |
| HDPE density | 950 g/L |
| CFRP density | 1600 g/L |
| GF density | 1800 g/L |
| CFRP tensile strength | 2550 MPa |

Table F.1: Parameters

[1] Technical Assessment of Compressed Hydrogen Storage Tank Systems for Automotive Applications, Appendix A

### Hydrogen volume and mass

From [1], a 258 L vessel contains 6 kg of hydrogen.

$$pV = mR_mT$$
$$R_mT = \frac{pV}{m} = \frac{35\ \text{MPa} \cdot 0.258\ \text{m}^3}{6\ \text{kg}} = 1.505\ (\text{m/s})^2$$

The recoverable hydrogen is:

$$m_R = m_f - m_e$$
$$\frac{p_fV_f}{m_f} = \frac{p_eV_e}{m_e}$$
$$m_R = m_f(1 - \frac{p_e}{p_f}) \rightarrow m_f = 1.061 \cdot m_R$$

where $R$ stands for *recoverable*, $f$ for *full*, and $e$ for *empty*. The volume necessary to store a mass $m_R$ of hydrogen is, then

$$V_{H_2} = \frac{m_fR_mT}{p_f} = \frac{1.061m_RR_mT}{p_f} = \frac{1.061 \cdot 1.505}{35}m_R = 45.62m_R\ [\text{L}]$$

The shape of the vessel has an area and volume:

$$A = 2\pi rL + 4\pi r^2 = 12\pi r^2 + 4\pi r^2 = 16\pi r^2$$
$$V = \frac{4}{3}\pi r^3 + \pi r^2L = \frac{4}{3}\pi r^3 + 6\pi r^3 = \frac{22}{3}\pi r^3$$

Given the volume, we can calculate the radius:

$$r = \sqrt[3]{\frac{3V}{22\pi}}$$

Once we have the radius of the inner volume, we can calculate the thickness of the CFRP layer.

$$t_{cf} = \frac{f_s p f_f r_{H_2}}{\sigma_{cf}\eta_T E_f}$$

where

- $f_s = 2.25$ is the security factor.
- $p = 35$ MPa is the nominal pressure
- $f_f = 1.25$ is the filling factor. Maximum pressure is 125% of nominal pressure to allow quicker fillings.
- $r_{H_2}$ is the inner radius.

- $\sigma_{cf} = 2550$ MPa is the carbon fiber tensile strength.
- $\eta_T = 82.5\%$ is the carbon fiber translation efficiency (the ratio between tensile strength of the composite and that of the fiber).
- $E_f = 0.85$ is the weld joint factor.

Once we know the thickness of the CF layer, we can calculate the mass of material for each layer as follows:

$$r \to A = 16\pi r^2 \to V_{material} = A \cdot t \to m = V_{material} \cdot \rho$$

The radius of each layer is:

$$r_i = r_{H_2} + \frac{t_i}{2}$$
$$r_{cf} = r_{H_2} + t_i + \frac{t_{cf}}{2}$$
$$r_o = r_{H_2} + t_i + t_{cf} + \frac{t_o}{2}$$

Then, the tank mass will be:

| Element | mass |
|---|---|
| $H_2$ | $m_f$ |
| Inner lining | $m_i$ |
| CFRP | $m_{cf}$ |
| Outter lining | $m_o$ |
| Foam | 5 kg |
| BOP | 19 kg |
| TOTAL | |

Table F.2: default

# Appendix G

# Hydro, wind, and solar energy

## G.1 Data

Table G.1: Parameters

| | Units | Value |
|---|---|---|
| Hydropower EROI[1] | – | 84 |
| Wind EROI[2] | – | 18 |
| Solar (PV) EROI[2] | – | 6–12* |
| Solar (Th) EROI[2] | – | 1.6–1.9* |
| Geothermal EROI[1] | – | 9 |
| Energy input $CO_2$e emissions[3]($e_{input}$) | kg/GJ | 71.39 |
| Energy input $CO_2$e depletion factor[3]($d_{input}$) | GJ/GJ | 0.959 |

[1]Source: 1
[2]Source: 2
[3]Source: 3
*The values used are the mean values

## G.2 Calculations

From the EROI expression, we can calculate the energy invested per energy produced:

$$\text{EROI} = \frac{E_{produced}}{E_{invested}} \rightarrow E_{invested} = E_{produced} \cdot \text{EROI}^{-1}$$

For a production of 1 GJe, the energy invested is, then

$$E_{invested} = \text{EROI}^{-1}$$

And the depletion and emission factors are

$$d_i = \text{EROI}^{-1} \cdot d_{input}$$
$$e_i = \text{EROI}^{-1} \cdot e_{input}$$

The results are listed in table 2.

Table G.2: Results

| Source | EROI | Depletion factor | Emission factor [kg $CO_2$e/GJ] |
|---|---|---|---|
| Hydro | 84 | 0.011 | 0.85 |
| Wind | 18 | 0.053 | 3.97 |
| Solar PV | 9 | 0.107 | 7.93 |
| Solar Th | 1.75 | 0.548 | 40.79 |
| Geothermal | 9 | 0.107 | 7.93 |

## G.3 References

1. EROI of different fuels and the implications for society

2. EROI of global energy resources

3. Annex: Energy inputs to the energy sector

# Appendix H

# Hydrogen

## H.1 Data

Table H.1: Energy and emissions of the production of 1 kg of $H_2$ in various hydrogen plants

| | Feedstock | Amount | Electricity[1] [kWh] | Process $CO_2$ |
|---|---|---|---|---|
| Coal gasification | Coal [kg] | 8.5 | +3.175 | 21.42 |
| Coal gasification CC[2] | Coal [kg] | 7.85 | -1.72 | 1.98 |
| Natural gas reforming | Gas [MJ] | 165 | -0.569 | 9.28 |
| Natural gas reforming CC[2] | Gas [MJ] | 164 | -1.405 | 0.93 |
| Ethanol reforming | Ethanol [L] | 8.29 | -0.49 | 0[3] |
| Water electrolysis | - | - | -54.3 | 0 |

[1]Electricity: +surplus -input
[2]CC: Carbon capture
[3]Ethanol process $CO_2$ emissions are subtracted because of its biogenic origin

Table H.2: Feedstock emissions and depletion factors

| Feedstock | Upstream emissions [kg $CO_2$e/GJ] | Upstream emissions [kg $CO_2$e/units] | Depletion factor |
|---|---|---|---|
| Coal [kg][1] | 15.93 | 0.441 | 1.167 |
| Natural gas [MJ] | 31.09 | 0.031 | 1.213 |
| Ethanol[2] [L] | 64.47 | 1.371 | 0.866 |
| Electricity [kWh] | 161.40 | 0.581 | 2.225 |

[1]Coal LHV= 27.7 MJ/kg
[2]Ethanol LHV= 21.27 MJ/L

Hydrogen LHV: 120.21 MJ/kg.

## H.2 Calculations

Total upstream emissions and depletion are calculated as follows:

$$e_{upstream} = \sum_j e^j_{upstream} \cdot q^j$$
$$D = \sum_j d^j \cdot q^j$$

Then, the energy output is the sum of the energetic value of hydrogen plus the electricity surplus—only coal gasification produces such surplus.

$$E_{output} = E_{\mathrm{H_2}} + E_{electricity}$$

Finally, the emission and depletion factor is calculated:

$$e = \frac{e_{upstream} + e_{process}}{E_{output}}$$
$$d = \frac{D}{E_{output}}$$

## H.3 Results

Table H.3: Results

| Method | Emission factor [kg $CO_2$e/GJ] | depletion factor |
|---|---|---|
| Coal gasification | 191.21 | 2.087 |
| Coal gasification CC | 53.60 | 2.226 |
| Natural gas reforming | 122.62 | 1.703 |
| Natural gas reforming CC | 56.94 | 1.748 |
| Ethanol reforming | 96.94 | 1.303 |
| Water electrolysis | 262.46 | 3.618 |

# Appendix I

# Natural gas

## I.1 Data

Table I.1: Some data for natural gas.

| Parameter | Units | Value |
|---|---|---|
| EROI | - | 18 |
| Distribution fugitive losses | % | 1.8 |
| Distribution point source losses | % | 3.0 |
| Distribution flared and fuel use gas | % | 8.4 |
| Natural gas $CO_2$e combustion emissions | kg/GJ | 55.78 |
| Energy input$CO_2$e emissions | kg/GJ | 71.30 |
| Energy input depletion factor | - | 0.959 |
| LHV | MJ/kg | 47.141 |
| Methane GWP factor | - | 25 |

## I.2 Combustion

Natural gas combustion has an emission factor of 55.78 kg $CO_2$e/GJ.

## I.3 Distribution

All distribution losses add up to 13.2%, i.e. distribution has an efficiency of $\eta_D = 86.8\%$. So, for every 1 GJ of natural gas consumed, the amount of natural gas that must be pumped into the distribution system is

$$E_{bd} = \frac{1 \text{ GJ}}{\eta_D} = 1.152 \text{ GJ}$$

Since wether point source losses are vented or flared is not stated in the documentation, it is assumed to be 50/50. Then, the amount of natural gas vented and flared is:

- Vented: 0.038 GJ (1.8% + 1.5%)
- Flared or fuel use: 0.114 GJ (1.5% + 8.4%)

Assuming that natural gas is pure methane, vented losses produce:

$$e_V = 0.038 \text{ GJ CH}_4 \frac{1 \text{ kg CH}_4}{47.141 \cdot 10^{-3} \text{ GJ}} \frac{25 \text{ kg CO}_2\text{e}}{1 \text{ kg CH}_4} = 20.16 \text{ kg CO}_2\text{e}$$

And flared and fuel use produce

$$e_{FF} = 0.114 \text{ GJ} \frac{55.78 \text{ kg CO}_2\text{e}}{\text{GJ}} = 6.36 \text{ kg CO}_2\text{e}$$

The total amount is:

$$e_{dist} = e_V + e_{FF} = 26.52 \text{ kgCO}_2\text{e}$$

## I.4 Extraction

The energy invested in the extraction of natural gas is:

$$\text{EROI} = \frac{E_{extracted}}{E_{invested}} \rightarrow E_{invested} = \frac{E_{extracted}}{\text{EROI}} = \frac{1.152 \text{ GJ}}{18} = 0.064 \text{ GJ}$$

This energy has a depletion factor of 0.959 and an emission factor of 71.39 kg $CO_2$e/GJ.

$$e_E = E_{invested} \cdot e_{input} = 4.57 \text{ kg CO}_2\text{e}$$
$$d_E = E_{invested} \cdot d_{input} = 0.061 \text{ GJ}$$

The total amount of non-renewable resources depleted for 1 GJ of natural gas to be used is then:

$$d = E_{extracted} + d_E = 1.213 \text{ GJ}$$

## I.5 Summary

Table I.2: Natural gas emission and depletion factors

| Parameter | Value | Units |
|---|---|---|
| Upstream emissions | 31.09 | kg $CO_2$e/GJ |
| Combustion emissions | 55.78 | kg $CO_2$e/GJ |
| Total emissions | 86.87 | kg $CO_2$e/GJ |
| Depletion factor | 1.213 | GJ/GJ |

# Appendix J

# Oil and coal

## J.1 Data

Table J.1: Emission factors for petroleum products and coal (source: 1)

| Fuel | Emission factor | Units |
|---|---|---|
| Coal | 96.21 | kg $CO_2$e/GJ |
| Petrol | 72.28 | kg $CO_2$e/GJ |
| Marine freight transportation | 0.029 | kg $CO_2$e/t-km |
| Marine freight transportation | 0.042 | kg $CO_2$/ton-mi |
| Residual fuel oil | 75.29 | kg $CO_2$e/GJ |
| Residual fuel oil | 11.27 | kg $CO_2$/gal |

From the major oil trade movements in 2004 (source: 2), and using map measurements, the mean distance oil travels before being used is estimated at 6964 km.

Refining efficiency values for different petroleum products are listed in table 2.

Table J.2: Refining efficiencies (source: 3)

| Product | Efficiency[1] [%] |
|---|---|
| Petrol | 83.3 |
| Residual fuel oil | 92.1 |

[1]With less desirable products excluded

The energy inputs to power have a depletion factor of $d_i = 0.959$ and an emission factor of $e_i = 71.39$ kg $CO_2$e/GJ (source: 4). The EROI of coal is estimated at 39, and that of oil is at 18 (source: 5).

Table J.3: Other parameters (source: 6)

| Parameter | Value | Units |
|---|---|---|
| Residual oil density | 3.752 | kg/gal |
| Residual oil LHV | 39.466 | MJ/kg |
| Crude oil LHV | 42.686 | MJ/kg |
| Coal LHV | 22.732 | MJ/kg |

## J.2 Refinery

From the efficiency data, we can calculate the amount of fuel used in the refinery:

$$\eta = \frac{E_{out}}{E_{in}} \rightarrow E_{in} = E_{out}(\eta^{-1} - 1)$$

The energy consumed in a refinery comes primarily from byproduct waste gas, natural gas, and byproduct petroleum coke. The data on emissions of byproducts is not specified, but they are surely higher than more refined products or natural gas. Therefore, we will use the residual fuel oil figures, which are a good trade-off between those byproducts and natural gas. Residual fuel oil has an emission factor of 75.29 kg $CO_2$e/GJ.

Table J.4: Refinery

| Fuel | After ref. [GJ] | Efficiency [%] | Fuel used [GJ] | Before ref. [GJ] | Emissions [kg $CO_2$e] |
|---|---|---|---|---|---|
| Petrol | 1 | 83.3 | 0.200 | 1.200 | 15.09 |
| Residual fuel oil | 1 | 92.1 | 0.086 | 1.086 | 6.46 |

## J.3 Distribution

Let $d_{ij}$ be the distance between regions $i$ and $j$, and $\phi_{ij}$ the flux of oil between those two regions, the weighted mean distance of global oil trade is:

$$D = \frac{\sum_{(i,j)} d_{ij} \cdot \phi_{ij}}{\sum_{(i,j)} \phi_{(ij)}} = 6964 \text{ km}$$

The distance for coal is assumed to be the same, due to lack of data. With a coefficient $K$ to compensate for last-mile delivering, and assuming that all transport is made by tanker, and that the tanker runs on residual fuel oil, the cost of transporting 1 t of oil or coal is then.

$$C_t = K \cdot D \cdot c$$

So, the cost of transporting 1 GJ of oil or coal is:

$$C_{\text{GJ}} = K \cdot D \cdot c \cdot \text{LHV}^{-1}$$

From the emissions figure of marine transport, we can estimate the energy cost of that transport.

$$c = \frac{e_{marine} \cdot \rho_{RFO} \cdot \mathrm{LHV}_{RFO}}{e_{RFO}} = 0.378 \text{ MJ/t-km}$$

Where $e_{marine} = 0.042$ kg $CO_2$/ton-mi $= 0.029$ kg $CO_2$/t-km is the emission factor for marine freight transportation, $\rho_{RFO}$ is the density of residual fuel oil, $\mathrm{LHV}_{RFO}$ is its low heating value, and $e_{RFO}$ is its $CO_2$ emission factor.

The expression used to evaluate the emissions derived from the transportation of oil and coal is:

$$\epsilon = K \cdot D \cdot e_{marine} \cdot \mathrm{LHV}^{-1}$$

With coefficients $K = 1.5$ for oil and $K = 1.2$ for coal—lower for coal is mostly consumed by power plants, rather than distributed to the final user—, the energy cost and emissions are:

Table J.5: Energy cost and emissions of coal and oil distribution

| Resource | Energy cost ($C$) [GJ/GJ] | Emissions ($\epsilon$) [kg $CO_2$e/GJ] |
|---|---|---|
| Oil | 0.093 | 7.10 |
| Coal | 0.139 | 10.66 |

Therefore, for each fuel we have:

Table J.6: Emissions and depletion due to distribution

| Fuel | After dist. [GJ] | $C$ [GJ/GJ] | $\epsilon$ [kg $CO_2$e/GJ] | Befor dist. [GJ] | Emissions [kg $CO_2$e] |
|---|---|---|---|---|---|
| Petrol | 1.200 | 0.093 | 7.10 | 1.312 | 8.52 |
| Residual fuel oil | 1.086 | 0.093 | 7.10 | 1.187 | 7.71 |
| Coal | 1.000 | 0.139 | 10.66 | 1.139 | 10.66 |

## J.4 Extraction

We can deduce the energy invested in the extraction from the EROI expression:

$$\mathrm{EROI} = \frac{E_{extracted}}{E_{invested}} \rightarrow E_{invested} = E_{extracted} \cdot \mathrm{EROI}^{-1}$$

The energy used in the extraction has a depletion factor of 0.959 and an emission factor of 71.39 kg $CO_2$e/GJ (source: 7.

In addition, mining operations—for coal—, and vented, flared, and fugitive gases also produce emissions. Coal mining operations generated 64.6 millions of tons of $CO_2$ equivalent out of a production of 891 millions of tons of coal in the US in 2013. With a $\mathrm{LHV}_{coal} = 22.732$ GJ/t, that is equivalent to $e_{mining} = 3.19$ kg $CO_2$e/GJ (consumed). In the case of oil, vented, flared and fugitive emissions (VFF) in the production of oil

Table J.7: Oil and coal extraction energy and emissions

| Fuel | After extr. [GJ] | EROI | Before extr. [GJ] | Emissions [kg $CO_2$e] |
|---|---|---|---|---|
| Petrol | 1.312 | 18 | 1.382 | 5.20 |
| Residual fuel oil | 1.187 | 18 | 1.250 | 4.71 |
| Coal | 1.139 | 39 | 1.167 | 2.08 |

are 40.8 g of $CH_4$, and 32.7 g of $CO_2$ per mmBtu of crude oil, which is equivalent to $e_{VFF} = 1.00$ kg $CO_2$e/GJ (extracted).

## J.5 Summary

Table J.8: Emission and depletion factors per GJ of fuel consumed

| Fuel | Upstream emissions [kg $CO_2$e] | Combustion emissions [kg $CO_2$e] | Total emisssions [kg $CO_2$e] | Depletion [GJ] |
|---|---|---|---|---|
| Petrol | 30.13 | 72.28 | 102.41 | 1.382 |
| Residual fuel oil | 20.06 | 75.29 | 95.35 | 1.250 |
| Coal | 15.93 | 96.21 | 112.14 | 1.167 |

## J.6 References

1. Annex: Estimation of fuel combustion emission factors.
2. Pipeline technology 2006 conference.
3. Estimation of Energy Efficiencies of U.S. Petroleum Refineries.
4. Annex: Depletion and emission factors of energy inputs to power.
5. EROI of global energy resources.
6. Biomass Energy Data Book (2011) - Appendix A: Lower and Higher Heating Values of Gas, Liquid and Solid Fuels.

# Appendix K

# Power plants

## K.1 Data

- Nuclear power plant construction cost: 6.5 $ (2000)/W (Source: 1).
- 1 $GW_e$ nuclear power plant energy cost of construction: 80 PJ (Source: 1).
- U.S. inflation from 2000 to 2013: 35.2% (Source: 2)

Table K.1: Construction data (Source: 3)

| Type | Cost [$(2013)/kW] | Mean Capacity [MW] | Capacity factor[1] [%] | Lifespan[2] [years] |
|---|---|---|---|---|
| Natural gas | 965 | 208 | 42.2 (US) | 40 |
| Biomass | 3495 | 13 | 56.5 (UK) | 40 |
| Coal[3] | 765 | 245 | 63.8 (US) | 40 |
| Oil | 765 | 18 | 7.8 (US) | 40 |

[1]Source: 4
[2]Assumed
[3]Coal powerplant construction cost assumed to be the same as petroleum liquids power plant.

Table K.2: Operation and maintenance data (source: 5)

| Type | Operation cost [$(2013)/MWh] | Maintenance [$(2013)/MWh] |
|---|---|---|
| Steam | 4.57 | 4.41 |
| Gas turbine and small scale | 2.56 | 2.80 |

## K.2 Calculations

The construction cost of a nuclear power plant is 6.5\$(2000), which is 8.79\$(2013). The energy intensity of construction is:

$$e_i = \frac{80 \text{ PJ}}{8.79 \text{ \$(2013)}} = 9.1 \text{ MJ/\$(2013)}$$

### K.2.1 Natural gas

Energy production over its lifetime:

$$E = 208 \text{ MW} \cdot 0.422 \cdot 40 \text{ yr} \frac{365 \text{ d}}{1 \text{ yr}} \frac{24 \text{ h}}{1 \text{ d}} = 30.76 \cdot 10^6 \text{ MWh}$$

Cost per unit of energy:

$$c_{const} = \frac{965 \cdot 10^3 \text{ \$/MW} \cdot 208 \text{ MW}}{30.76 \cdot 10^6 \text{ MWh}} = 6.53 \text{ \$/MWh}$$

Total energy cost:

$$C_e = (c_{const} + c_{op} + c_m) \cdot e_i = (6.53 + 2.56 + 2.8) \cdot 9.1 = 108.20 \text{ MJ/MWh}$$

### K.2.2 Coal

Energy production over its lifetime:

$$E = 245 \text{ MW} \cdot 0.638 \cdot 40 \text{ yr} \frac{365 \text{ d}}{1 \text{ yr}} \frac{24 \text{ h}}{1 \text{ d}} = 54.77 \cdot 10^6 \text{ MWh}$$

Cost per unit of energy:

$$c_{const} = \frac{765 \cdot 10^3 \text{ \$/MW} \cdot 245 \text{ MW}}{54.77 \cdot 10^6 \text{ MWh}} = 3.42 \text{ \$/MWh}$$

Total energy cost:

$$C_e = (c_{const} + c_{op} + c_m) \cdot e_i = (3.42 + 4.57 + 4.41) \cdot 9.1 = 112.84 \text{ MJ/MWh}$$

### K.2.3 Biomass

Energy production over its lifetime:

$$E = 18 \text{ MW} \cdot 0.566 \cdot 40 \text{ yr} \frac{365 \text{ d}}{1 \text{ yr}} \frac{24 \text{ h}}{1 \text{ d}} = 3.56 \cdot 10^6 \text{ MWh}$$

Cost per unit of energy:

$$c_{const} = \frac{3495 \cdot 10^3 \text{ \$/MW} \cdot 13 \text{ MW}}{3.56 \cdot 10^6 \text{ MWh}} = 6.96 \text{ \$/MWh}$$

Total energy cost:

$$C_e = (c_{const} + c_{op} + c_m) \cdot e_i = (6.96 + 2.56 + 2.8) \cdot 9.1 = 112.11 \text{ MJ/MWh}$$

### K.2.4 Oil

Energy production over its lifetime:

$$E = 18\text{ MW} \cdot 0.078 \cdot 40\text{ yr}\frac{365\text{ d}}{1\text{ yr}}\frac{24\text{ h}}{1\text{ d}} = 4.92 \cdot 10^5\text{ MWh}$$

Cost per unit of energy:

$$c_{const} = \frac{765 \cdot 10^3\text{ \$/MW} \cdot 18\text{ MW}}{4.92 \cdot 10^5\text{ MWh}} = 27.99\text{ \$/MWh}$$

Total energy cost:

$$C_e = (c_{const} + c_{op} + c_m) \cdot e_i = (27.99 + 2.56 + 2.80) \cdot 9.1 = 303.47\text{ MJ/MWh}$$

### K.2.5 Summary

| Powerplant type | Construction, operation and maintenance cost [MJ/MWh] |
|---|---|
| Natural gas | 108.20 |
| Coal | 112.84 |
| Biomass | 112.11 |
| Oil | 303.47 |

Table K.3: default

## K.3 References

1. Stormsmith, Nuclear Power–The energy balance.

2. http://www.usinflationcalculator.com

3. www.eia.gov/electricity/generatorcosts

4. https://en.wikipedia.org/wiki/Capacity_factor

5. www.eia.gov/electricity/annual/html/epa_08_04.html

# Appendix L

# Social cost of carbon

## L.1 Data

Table L.1: Social cost of carbon [$2007/t$CO_2$] (source:1)

| | Discount rate [%] | | | |
|---|---|---|---|---|
| Year | 5.0 (Avg) | 3.0 (Avg) | 2.5 (Avg) | 3.0 (95th) |
| 2010 | 11 | 32 | 51 | 89 |
| 2015 | 11 | 37 | 57 | 109 |
| 2020 | 12 | 43 | 64 | 128 |
| 2025 | 14 | 47 | 69 | 143 |
| 2030 | 16 | 52 | 75 | 159 |
| 2035 | 19 | 56 | 80 | 175 |
| 2040 | 21 | 61 | 86 | 191 |
| 2045 | 24 | 66 | 92 | 206 |
| 2050 | 26 | 71 | 97 | 220 |

## L.2 Calculations

The value of one US dollar of 2005 and 2007 in 2020 depends on the discount rate used. Using the inflation data from 2005 to 2015 and the discount rate from 2015 to 2020, the cumulative inflation is:

The energy intensity shows a clear linear trend. The projected energy intensity in the year 2020 is 0.136 koe/$2005, which is equivalent to 5.69 MJ/$2005. Converting $2005 to $2020, we have:

So, for the four possible values of the social cost of carbon in 2020, we can calculate the equivalent to energy:

Table L.2: Global energy intensity and US inflation

| Year | Energy intensity[1] [koe/$2005] | Inflation[2] [%] |
|---|---|---|
| 2005 | 0.180 | 3.40 |
| 2006 | 0.176 | 3.20 |
| 2007 | 0.172 | 2.80 |
| 2008 | 0.168 | 3.80 |
| 2009 | 0.167 | −0.40 |
| 2010 | 0.166 | 1.60 |
| 2011 | 0.162 | 3.20 |
| 2012 | 0.159 | 2.10 |
| 2013 | 0.157 | 1.50 |
| 2014 | 0.153 | 1.60 |
| 2015 | 0.149 | 0.10 |

[1]Source: 2

[2]Source: 3

Table L.3: Cumulative inflation rate

| | Cumulative inflation rate [%] | |
|---|---|---|
| Discount rate [%] | 2005–2020 | 2007–2020 |
| 2,50 | 37,13 | 29,26 |
| 3.00 | 40,51 | 32,45 |
| 5.00 | 54,69 | 45,81 |

## L.3 References


1. Technical Update of the Social Cost of Carbon for Regulatory Impact Analysis– Under Executive Order 12866

2. https://yearbook.enerdata.net/#energy-intensity-GDP-by-region.html

3. http://www.usinflationcalculator.com/inflation/historical-inflation-rates/

Table L.4: Energy intensity

| Discount rate [%] | 2.5 | 3.0 | 5.0 |
|---|---|---|---|
| Energy intensity [MJ/$2020] | 4.15 | 4.05 | 3.68 |

Table L.5: Energy equivalent to SCC

| Discount rate [%] | SCC [$2007/t$CO_2$] | SCC [$2020/t$CO_2$] | Energy intensity [MJ/$2020] | Energy [MJ] |
|---|---|---|---|---|
| 2.50 (Avg) | 12.00 | 15.51 | 4.15 | 64.36 |
| 3.00 (Avg) | 43.00 | 56.95 | 4.05 | 230.63 |
| 5.00 (Avg) | 64.00 | 93.32 | 3.68 | 343.26 |
| 3.00 (95th) | 128.00 | 169.53 | 4.05 | 686.51 |

# Appendix M

# Small vehicle weights

## M.1 Data

## M.2 Calculations

The following operations have been performed to the data in order to obtain the kerb weight:

$$m_0 = m - V_{fuel}\, \rho_{fuel} - m_{driver} \tag{M.1}$$

Then, a simple linear regression is performed between kerb weight and power to obtain an approximation of the base weight and the powertrain specific power.

## M.3 Results

The data is fitted to the curve described by [EQUATION].

$$m = p_s^{-1}\, P + m_0 \tag{M.2}$$

where $p_s$ is the specific power. The results are those of [TABLE].

The fit is not very good (adjusted $R^2 = 0.5751$), but it is satisfactory as an approximation. The values used are:

## M.4 References

[1] Retrieved from http://www.coches.net on 27/4/2016

Table M.1: Data [1]

| Car model | Power $P$ [HP] | Mass $m$ [kg] | Fuel capacity $V_{fuel}$ [L] |
|---|---|---|---|
| C1 68 | 69 | 875 | 35 |
| C1 82 | 82 | 865 | 35 |
| Ford Ka | 69 | 940 | 35 |
| Skoda Citigo 60 | 60 | 840 | 35 |
| Skoda Citigo 75 | 75 | 829 | 35 |
| VW Up 60 | 60 | 929 | 35 |
| VW Up 75 | 75 | 929 | 35 |
| Fiat 500 1.2 | 69 | 865 | 35 |
| Fiat 500 0.9 | 105 | 940 | 35 |
| Mini One | 102 | 1165 | 40 |
| Mini Cooper | 136 | 1160 | 40 |
| Mini Cooper S | 192 | 1235 | 44 |
| Mini JCW | 231 | 1280 | 44 |
| Opel Adam 1.2 | 70 | 1086 | 35 |
| Opel Adam 1.4 | 100 | 1135 | 35 |
| Opel Adam 1.0 | 115 | 1156 | 35 |
| Opel Adam 1.4 NEH | 150 | 1178 | 35 |
| Renault twingo 70 | 70 | 865 | 35 |
| Renault twingo 90 | 90 | 943 | 35 |
| Seat Mii 60 | 60 | 929 | 35 |
| Seat Mii 75 | 75 | 929 | 35 |
| Toyota Aygo | 69 | 855 | 35 |
| Smart Fortwo 45 | 61 | 750 | 33 |
| Smart Fortwo 52 | 71 | 750 | 28 |
| Smart Fortwo 62 | 84 | 770 | 33 |
| Smart Fortwo 66 | 90 | 900 | 28 |
| Smart Fortwo Brabus | 102 | 795 | 33 |

Table M.2: Other parameters

| Parameter | Value |
|---|---|
| Driver mass [kg] | 75 |
| Petrol density [kg/L] | 0.747 |

Table M.3: default

| | | 95% confidence bounds | |
|---|---|---|---|
| Coefficient | Value | Min | Max |
| $p_s^{-1}$ [kg/HP] | 2.87 | 1.887 | 2.852 |
| $m_0$ [kg] | 588.5 | 488.2 | 688.8 |

Table M.4: Results

| Parameter | Symbol | Units | Value |
|---|---|---|---|
| Base weight | $m_0$ | kg | 500 |
| Specific power | $p_s$ | W/kg | 256 |